

EXAMINATION OF THE NATURE OF
THE BIANCHI TYPE COSMOLOGICAL SINGULARITIES.

Piotr Dzierżak

Theoretical Physics Department
Institute for Nuclear Studies



PhD Thesis

2010

SUPERVISED BY PROF. WŁODZIMIERZ PIECHOCKI

Abstract

We present quantum (and classical) Bianchi I model, with free massless scalar field, of the Universe. Our model may be treated as the simplest prototype of the quantum BKL (Belinskii-Khalatnikov-Lifshitz) scenario. The quantization is done by making use of the nonstandard Loop Quantum Cosmology (LQC). Since the method is quite new, we present in details its motivation and the formalism. To make the nonstandard method easily understandable, we include its application to the FRW model. We solve the Hamiltonian constraint of the theory at the classical level and find elementary observables. Physical compound observables are defined in terms of elementary ones. We find that classical Big Bang singularity is replaced by quantum Big Bounce transition due to modification of classical theory by holonomy around a loop with finite size. The energy density of matter fields at the Big Bounce depends on a free parameter λ , which value is expected to be determined from future cosmological observations. The phase space is divided into two distinct regions: Kasner-like and Kasner-unlike. We use the elementary observables to quantize volume and directional volume operators in both cases. Spectra of these operators are bounded from below and discrete, and depend on λ . The discreteness may imply a foamy structure of spacetime at semi-classical level. At the quantum level an evolution of the model is generated by the so-called true Hamiltonian. This enables introducing a time parameter valued in the set of all real numbers.

*To someone without whom this Thesis
would be never finished*

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Acknowledgements

I would like to thank Prof. Włodzimierz Piechocki, my supervisor, who introduced me to the problems and methods of Quantum Cosmology and with whom I shared a pleasure of joint scientific investigations.

I am grateful to my dear friend Dr Przemysław Małkiewicz, who helped me understanding some intriguing mathematical problems.

Warsaw, December 30, 2010

Piotr Dzierżak

This Thesis is based on the following author's papers:

- [1] P.Dz., Jacek Jezierski, Przemysław Małkiewicz and Włodzimierz Piechocki,
“The minimum length problem of loop quantum cosmology”, *Acta Phys. Polon.* **41** (2010) 717, arXiv:0810.3172.
- [2] P.Dz., Przemysław Małkiewicz and Włodzimierz Piechocki,
“Turning Big Bang into Big Bounce: I. Classical Dynamics”, *Phys. Rev. D* **80**, 104001 (2009), arXiv:0907.3436.
- [3] P.Dz. and Włodzimierz Piechocki,
“Bianchi I model in terms of non-standard LQC: Classical dynamics”, *Phys. Rev. D* **80**, 124033 (2009), arXiv:0909.4211.
- [4] P.Dz. and Włodzimierz Piechocki,
“Bianchi I model of the universe in terms of nonstandard LQC”, *Ann. Phys.* **19** (2010) 290.
- [5] Przemysław Małkiewicz, Włodzimierz Piechocki and P.Dz.,
“Bianchi I model in terms of nonstandard loop quantum cosmology: Quantum dynamics.”, *Class. Quant. Grav.* **28**, 085020 (2011), arXiv:1010.2930.

Introduction

It results from cosmological observations that the Universe emerged from a state characterized by extremely high density of matter fields called Big Bang or cosmological singularity [1, 2, 3, 4]. The observational data are in comparatively good agreement with calculations obtained within the standard cosmological models (SCM). The latter is based on General Relativity (GR), and includes dark matter, dark energy and the inflation transition. However, SCM provides a phenomenological description. Deep understanding of the cosmological data, in particular of an early Universe requires an elementary quantum theory being able to explain creation of spacetime filled with matter fields.

Probably, the best starting point for finding such a theory is quantization of the BKL (Belinskii, Khalatnikov, Lifshitz) scenario [5, 6, 7]. First of all, it is clear from this scenario that a general solution of the Einstein equation with the cosmological singularity does exist. By this term we mean a singularity in time on spacelike hypersurface characterized by blowing up the curvature invariants together with diverging energy densities of matter fields. The BKL solution of GR is general and stable. By general we mean containing a non-zero measure subset of all initial conditions. Stability means that no infinitesimal perturbations of initial conditions is able to change the singular character of the solution.

Secondly the BKL scenario says that in asymptotic vicinity of the singularity this general solution has complicated oscillatory behavior of chaotic character. There is considerable support for this scenario both from analytical [8, 9] and numerical [10] investigations. What is important in the BKL the dynamics at any spatial point can be approximated by that of the homogeneous (but in general non-isotropic) models which are called Bianchi models [5, 6, 7].

In the BKL scenario, time derivatives of gravitational field is shown to dominate over spatial derivatives for long stretches of time. During such periods called Kasner epochs, an evolution of gravitational field may be approximated by the Bianchi I model [11].

In each Kasner epoch the Universe is approximated by the Bianchi I metric with some specific set of parameters k_i satisfied equations $\sum_{i=1}^3 k_i = 1$ and $\sum_{i=1}^3 k_i^2 + k_\phi^2 = 1$ where k_ϕ describes density of matter fields. There exist two classes of solutions. The first, called Kasner-like, one of k_i has different sign than two others. It means that the Universe contracts in two directions and expands in the third. The second one, called Kasner-unlike, all the parameteres have the same sign, which means that there is a contraction in every direction. This is not the end, because from time to time there occur short periods in the evolution when spatial derivatives of gravitational field dominate over time derivatives, which lead to the transitions between Kasner epochs. In each transition the set of the parameters k_i characterizing the specific Bianchi I model changes to another one. Dynamics of the transitions can be modelled by the Bianchi II time evolution [12].

In the BKL scheme, the Universe may undergo an infinite number of chaotic-like transitions (depending on equation of state of matter fields) from one Kasner epoch

to another, and finally collapse to a singularity in a finite proper time [8, 9]. It is clear that before the system approaches the singularity, the spacetime curvature acquires the Planck scale so the classical scenario cannot be trusted.

It is clear that, according to the BKL scenario, there are two basic steps in understanding of an early Universe. The first one means the construction of the quantum Bianchi I model of the Universe [13], and the second one means finding the quantum Bianchi II model. This Thesis is devoted to the first task.

Quantization in this Thesis is based on the so-called nonstandard Loop Quantum Cosmology (LQC) which is an alternative to the standard Loop Quantum Cosmology. The difference between them will be discussed later. The standard LQC is a cosmological counterpart of Loop Quantum Gravity (LQG) and is obtained by symmetry reduction of LQG, which as a field theory has infinite number of degrees of freedom [14]. On the other hand LQG is a non-perturbative theory being today one of the most promising candidate to the theory of unification GR with quantum physics. Both geometry and matter are dynamical and described by quantum mechanics. In LQG there is no background spacetime [15].

This Thesis is organized as follows:

Chapter 1 is an introduction and contains main features of both existing LQC methods, namely the standard and the nonstandard. In Section 1 of this chapter we describe formalism of the standard LQC concentrating mainly on its successes in resolving the cosmological singularity. Section 2 contains a motivation for another LQC method, which underlines the Thesis. In Section 3 we describe this method, called the nonstandard LQC and make a comparison between these two methods. In Section 4 we present an application of the nonstandard LQC to the simplest cosmological

model, namely FRW. At the classical level we show the occurrence of Big Bounce. At the quantum level particular attention is paid to volume and energy density operators. Spectra of these operators are analyzed in details.

Chapter 2 is the main part of the Thesis. Here we present an application of nonstandard LQC to the Bianchi I cosmological model. Section 1 is devoted to calculations done on the classical level, which mean solving the equations of motions and finding the algebra of elementary observables. In Section 2 we make, before quantizing, some comfortable redefinitions and, what is more important, analyze structure of the phase space. So-called true Hamiltonian is introduced. In Section 3 we face the quantization in Kasner-like and Kasner-unlike cases. Particular attention is paid to the volume operator and the problem of an evolution.

In Conclusions we make summary of all the results.

Appendix A presents curvature of connection expressed in terms of holonomies. Classification of phase space in terms of observables includes Appendix B. Some ambiguities in quantization are discussed in Appendix C.

Chapter 1

Loop Quantum Cosmology

1.1 Formalism of standard LQC

1.1.1 Basic facts

By the standard LQC one means LQC that is strongly inspired by LQG [15, 16, 17]. The inspiration consists mainly in applying the two ingredients of LQG: (i) modification of the curvature of connection by loop geometry, and (ii) making use of the holonomy-flux variables. The construction of LQC has been carried out by mimicry of the construction of LQG.

The LQC was firstly applied to quantization of FRW model as FRW is the most common model in cosmology and astrophysics today. This field is not very old, because the first papers appeared less than 10 years ago [18, 19]. Since then more than 100 papers have been written. Amongst the most important are [14, 20, 21, 22, 23]. We recommend also a few review articles [24, 25, 26, 27].

The standard LQC [14, 20] means basically the Dirac method of quantization, which begins with quantization of the kinematical phase space followed by imposition of constraints of the gravitational system in the form of operators acting on a

kinematical Hilbert space. Then, one must solve these constraints which means finding kernels of the operators. The kernels are used to identify the physical Hilbert space.

1.1.2 Big Bounce

The most important result obtained within the standard LQC is that the classical Big Bang (and also the Big Crunch) is replaced by the quantum Big Bounce due to strong quantum effects at the Planck scale [24, 25, 26]. The result was obtained for FRW models with $k = 0$ and $k = 1$ and for Bianchi I model [24]. It was done using analytical and numerical methods [18, 22, 28]. In all these models the role of internal time was played by a scalar field which enables interpreting the Hamiltonian constraint as an evolution equation. Singularity is resolved in the sense that observables like energy density of matter which classically diverge, are represented by operators bounded from above on the states (vectors of the physical Hilbert space) which are semi-classical asymptotically [22]. It is suggested in [23] that the bounce may occur for the states which are more general than semi-classical at late times, which demonstrates robustness of LQC results. Quantum evolution, described by (1.2.24), is deterministic across the bounce region. An universe undergoes a bounce during the evolution from an epoch before the Big Bang to an epoch after the Big Bang, so on the “other side” of the bounce there is also a universe [25]. These are main highlights of LQC (see, e.g. [27] for a complete list).

There exists an alternative to the standard LQC approach called the nonstandard LQC, which is presented and applied in the rest of the Thesis.

1.2 Motivation for nonstandard LQC

1.2.1 Hamiltonian

The gravitational part of the classical Hamiltonian, H_g , in GR is a linear combination of the first-class constraints, and reads [14, 15, 16, 17, 20]

$$H_g := \int_{\Sigma} d^3x (N^i C_i + N^a C_a + NC), \quad (1.2.1)$$

where Σ is the spacelike part of spacetime $\mathbb{R} \times \Sigma$, (N^i, N^a, N) denote Lagrange multipliers, (C_i, C_a, C) are the Gauss, diffeomorphism and scalar constraints. In our notation $(a, b = 1, 2, 3)$ are spatial, and $(i, j, k = 1, 2, 3)$ internal $SU(2)$ indices. The constraints must satisfy a specific algebra.

For flat FRW model with massless scalar field we can rewrite the gravitational part of the classical Hamiltonian, having fixed local gauge and diffeomorphism freedom, in the form (see, e.g. [22])

$$H_g = -\gamma^{-2} \int_{\mathcal{V}} d^3x Ne^{-1} \varepsilon_{ijk} E^{aj} E^{bk} F_{ab}^i, \quad (1.2.2)$$

where γ is the Barbero-Immirzi parameter, $\mathcal{V} \subset \Sigma$ is an elementary cell, Σ is spacelike hyper-surface, N denotes the lapse function, ε_{ijk} is the alternating tensor, E_i^a is a densitized vector field, $e := \sqrt{|\det E|}$, and where F_{ab}^i is the curvature of an $SU(2)$ connection A_a^i .

The resolution of the singularity, obtained within LQC, is based on rewriting the curvature F_{ab}^k in terms of holonomies around loops. The curvature F_{ab}^k may be determined [22] by making use of the formula (see the Appendix A)

$$F_{ab}^k = -2 \lim_{Ar \square_{ij} \rightarrow 0} Tr \left(\frac{h_{\square_{ij}}^{(\lambda)} - 1}{\lambda^2 V_o^{2/3}} \right) \tau^k {}^o \omega_a^i {}^o \omega_a^j, \quad (1.2.3)$$

where

$$h_{\square_{ij}}^{(\lambda)} = h_i^{(\lambda)} h_j^{(\lambda)} (h_i^{(\lambda)})^{-1} (h_j^{(\lambda)})^{-1} \quad (1.2.4)$$

is the holonomy of the gravitational connection around the square loop \square_{ij} , considered over a face of the elementary cell, each of whose sides has length $\lambda V_o^{1/3}$ with respect to the flat fiducial metric ${}^o q_{ab} := \delta_{ij} {}^o \omega_a^i {}^o \omega_a^j$; fiducial triad ${}^o e_k^a$ and cotriad ${}^o \omega_a^k$ satisfy ${}^o \omega_a^i {}^o e_j^a = \delta_j^i$; the spatial part of the FRW metric is $q_{ab} = a^2(t) {}^o q_{ab}$; $Ar \square_{ij}$ denotes the area of the square; $V_o = \int_{\mathcal{V}} \sqrt{{}^o q} d^3x$ is the fiducial volume of \mathcal{V} . Because its value is for our analysis not essential, we set $V_0 = 1$. Here we would like to emphasize that (1.2.3) is exact iff $\lambda = 0$, which is not our case.

The holonomy along straight edge ${}^o e_k^a \partial_a$ of length $\lambda V_0^{1/3}$ reads

$$h_k^{(\lambda)}(c) = \mathcal{P} \exp \left(\int_0^{\lambda V_0^{1/3}} \tau_{(k)} A_a^{(k)} dx^a \right) = \exp(\tau_k \lambda c) = \cos(\lambda c/2) \mathbb{I} + 2 \sin(\lambda c/2) \tau_k, \quad (1.2.5)$$

where $\tau_k = -i\sigma_k/2$ (σ_k are the Pauli spin matrices) and \mathcal{P} denotes the path ordering symbol. Equation (1.2.5) presents the holonomy calculated in the fundamental, $j = 1/2$, representation of $SU(2)$.

Making use of (1.2.2), (1.2.3) and the so-called Thiemann identity [16]

$$\varepsilon_{ijk} e^{-1} E^{aj} E^{bk} = \frac{sgn(p)}{2\pi G \gamma \lambda} \sum_k {}^o \varepsilon^{abc} {}^o \omega_c^k Tr \left(h_k^{(\lambda)} \{(h_k^{(\lambda)})^{-1}, V\} \tau_i \right) \quad (1.2.6)$$

leads to H_g in the form

$$H_g = \lim_{\lambda \rightarrow 0} H_g^{(\lambda)}, \quad (1.2.7)$$

where

$$H_g^{(\lambda)} = -\frac{sgn(p)}{2\pi G \gamma^3 \lambda^3} \sum_{ijk} N \varepsilon^{ijk} Tr \left(h_i^{(\lambda)} h_j^{(\lambda)} (h_i^{(\lambda)})^{-1} (h_j^{(\lambda)})^{-1} h_k^{(\lambda)} \{(h_k^{(\lambda)})^{-1}, V\} \right), \quad (1.2.8)$$

and where $V = |p|^{\frac{3}{2}} = a^3$ is the volume of the elementary cell \mathcal{V} .

The connection A_a^k and the density weighted triad E_k^a which occurs in (1.2.6) is determined by the conjugate variables c and p as follows: $A_a^k = {}^o\omega_a^k c$ and $E_k^a = {}^o e_k^a \sqrt{q_o} p$, where $c = \gamma \dot{a}$ and $|p| = a^2$.

It should be noticed that in this section we use the “old” quantization scheme [21]. There exists also the “improved” scheme $\bar{\mu} = \sqrt{\frac{1}{|p|}} \lambda$ described in [22] and used in section “Application” of this Thesis. It has serious advantages and is now commonly used by LQC community. However, obtained results concern both methods [29].

The classical total Hamiltonian for FRW universe with a massless scalar field, ϕ , reads

$$H = H_g + H_\phi \approx 0, \quad (1.2.9)$$

where H_g is defined by (1.2.7) and where sign “ \approx ” reminds that H is a constraint of the system. The Hamiltonian of the scalar field is known to be: $H_\phi = N p_\phi^2 |p|^{-\frac{3}{2}} / 2$, where ϕ and p_ϕ are the elementary variables satisfying $\{\phi, p_\phi\} = 1$. The relation $H \approx 0$ defines the physical phase space of considered gravitational system with constraints.

1.2.2 Quantization

In the Dirac quantization [30, 31] we find a kernel of the quantum operator \hat{H} corresponding to H , i.e.

$$\hat{H}\Psi = 0, \quad (1.2.10)$$

since the classical Hamiltonian is a constraint of the system, and try to define a scalar product on the space of solutions to (1.2.10). This gives a starting point for the determination of the physical Hilbert space \mathcal{H}_{phys} .

Kinematics

The classical elementary functions satisfy the relation

$$\{p, N_\lambda\} = -i \frac{4\pi G \gamma}{3} \lambda N_\lambda, \quad (1.2.11)$$

where G is the Newton constant. Quantization of the algebra (1.2.11) is done by making use of the prescription

$$\{\cdot, \cdot\} \longrightarrow \frac{1}{i\hbar} [\cdot, \cdot]. \quad (1.2.12)$$

The basis of the representation space is chosen to be the set of eigenvectors of the momentum operator [14] and is defined by

$$\hat{p} |\mu\rangle = \frac{4\pi\gamma l_p^2}{3} \mu |\mu\rangle, \quad \mu \in \mathbb{R}, \quad (1.2.13)$$

where $l_p^2 = G\hbar$. The operator corresponding to N_λ acts as follows

$$\hat{N}_\lambda |\mu\rangle = |\mu + \lambda\rangle. \quad (1.2.14)$$

The quantum algebra corresponding to (1.2.11) reads

$$\frac{1}{i\hbar} [\hat{p}, \hat{N}_\lambda] |\mu\rangle = -i \frac{4\pi G \gamma}{3} \lambda \hat{N}_\lambda |\mu\rangle. \quad (1.2.15)$$

The carrier space, \mathcal{F}_g , of the representation (1.2.15) is the space spanned by $\{|\mu\rangle, \mu \in \mathbb{R}\}$ with the scalar product defined as

$$\langle \mu | \mu' \rangle := \delta_{\mu, \mu'}, \quad (1.2.16)$$

where $\delta_{\mu, \mu'}$ denotes the Kronecker delta.

The completion of \mathcal{F}_g in the norm induced by (1.2.16) defines the Hilbert space $\mathcal{H}_{kin}^g = L^2(\mathbb{R}_{Bohr}, d\mu_{Bohr})$, where \mathbb{R}_{Bohr} is the Bohr compactification of the real line

and $d\mu_{Bohr}$ denotes the Haar measure on it [14]. \mathcal{H}_{kin}^g is the kinematical space of the gravitational degrees of freedom. The kinematical Hilbert space of the scalar field is $\mathcal{H}_{kin}^\phi = L^2(\mathbb{R}, d\phi)$, and the operators corresponding to the elementary variables are

$$(\hat{\phi}\psi)(\phi) = \phi\psi(\phi), \quad \hat{p}_\phi\psi = -i\hbar \frac{d}{d\phi}\psi. \quad (1.2.17)$$

The kinematical Hilbert space of the gravitational field coupled to the scalar field is defined to be $\mathcal{H}_{kin} = \mathcal{H}_{kin}^g \otimes \mathcal{H}_{kin}^\phi$.

Dynamics

The resolution of the singularity [14, 20, 21, 22, 23] is mainly due to the peculiar way of defining the quantum operator corresponding to H_g . Let us consider this issue in more details.

Using the prescription $\{\cdot, \cdot\} \rightarrow \frac{1}{i\hbar}[\cdot, \cdot]$ and specific factor ordering of operators, one obtains from (1.2.8) a quantum operator corresponding to $H_g^{(\lambda)}$ in the form [14]

$$\hat{H}_g^{(\lambda)} = \frac{i \operatorname{sgn}(p)}{2\pi l_p^2 \gamma^3 \lambda^3} \sum_{ijk} \varepsilon^{ijk} \operatorname{Tr} \left(\hat{h}_i^{(\lambda)} \hat{h}_j^{(\lambda)} (\hat{h}_i^{(\lambda)})^{-1} (\hat{h}_j^{(\lambda)})^{-1} \hat{h}_k^{(\lambda)} \{(\hat{h}_k^{(\lambda)})^{-1}, \hat{V}\} \right). \quad (1.2.18)$$

One can show [14] that (1.2.18) can be rewritten as

$$\hat{H}_g^{(\lambda)} |\mu\rangle = \frac{3}{8\pi\gamma^3\lambda^3 l_p^2} (V_{\mu+\lambda} - V_{\mu-\lambda}) (|\mu+4\lambda\rangle - 2|\mu\rangle + |\mu-4\lambda\rangle), \quad (1.2.19)$$

where $|\mu\rangle$ is an eigenstate of \hat{p} defined by (1.2.13), and where V_μ is an eigenvalue of the volume operator corresponding to $V = |p|^{3/2}$ which reads

$$\hat{V} |\mu\rangle = \left(\frac{4\pi\gamma|\mu|}{3} \right)^{3/2} l_p^3 |\mu\rangle =: V_\mu |\mu\rangle. \quad (1.2.20)$$

The quantum operator corresponding to H_g is defined to be [14, 21]

$$\hat{H}_g := \hat{H}_g^{(\lambda)} |_{\lambda=\mu_o}, \quad \text{where } 0 < \mu_o \in \mathbb{R}. \quad (1.2.21)$$

Comparing (1.2.21) with (1.2.7), and taking into account (1.2.3) one can see that the area of the square \square_{ij} is not shrunk to zero, as required in the definition of the classical curvature (1.2.3), but determined at the finite value of the area.

The mathematical justification proposed in [14, 21] for such regularization is that one cannot define the local operator corresponding to the curvature F_{ab}^k because the 1-parameter group \hat{N}_λ is not weakly continuous at $\lambda = 0$ in \mathcal{F}_g (dense subspace of \mathcal{H}_{kin}^g). Thus, the limit $\lambda \rightarrow 0$ of $\hat{H}_g^{(\lambda)}$ does not exist. To determine μ_o one proposes in [14, 21, 22] the procedure which is equivalent to the following: We find that the area of the face of the cell \mathcal{V} orthogonal to specific direction is $Ar = |p|$. Thus the eigenvalue problem for the corresponding kinematical operator of an area $\widehat{Ar} := |\hat{p}|$, due to (1.2.13), reads

$$\widehat{Ar} |\mu\rangle = \frac{4\pi\gamma l_p^2}{3} |\mu| |\mu\rangle =: ar(\mu) |\mu\rangle, \quad \mu \in \mathbb{R}, \quad (1.2.22)$$

where $ar(\mu)$ denotes the eigenvalue of \widehat{Ar} corresponding to the eigenstate $|\mu\rangle$. On the other hand, it is known that in LQG the kinematical area operator has discrete eigenvalues [32, 33] and the smallest nonzero one, called an area gap Δ , is given by $\Delta = 2\sqrt{3}\pi\gamma l_p^2$. To identify μ_o one postulates in [21] that μ_o is such that $ar(\mu_o) = \Delta$, which leads to $\mu_o = 3\sqrt{3}/2$. It is argued [14, 21, 22, 23] that one cannot squeeze a surface to the zero value due to the existence in the universe of the minimum quantum of area. This completes the justification for the choice of the expression defining the quantum Hamiltonian (1.2.21) offered by LQC.

It is interesting to notice that for the model considered here (defined on one-dimensional constant lattice) the existence of the minimum area leads to the reduction of the non-separable space \mathcal{F}_g to its separable subspace. It is so because due to (1.2.14)

we have

$$\hat{N}_{\mu_o} |\mu\rangle = |\mu + \mu_o\rangle, \quad (1.2.23)$$

which means that the action of this operator does not lead outside of the space spanned by $\{|\mu + k\mu_o\rangle, k \in \mathbb{Z}\}$, where $\mu \in \mathbb{R}$ is fixed.

Finally, one can show (see, e.g. [14, 21]) that the equation for quantum dynamics, corresponding to (1.2.10), reads

$$B(\mu) \partial_\phi^2 \psi(\mu, \phi) - C^+(\mu) \psi(\mu + 4\mu_o, \phi) - C^-(\mu) \psi(\mu - 4\mu_o, \phi) - C^0(\mu) \psi(\mu, \phi) = 0, \quad (1.2.24)$$

where

$$B(\mu) := \left(\frac{2}{3\mu_o}\right)^6 [|\mu + \mu_o|^{3/4} - |\mu - \mu_o|^{3/4}]^6, \quad C^0(\mu) := -C^+(\mu) - C^-(\mu), \quad (1.2.25)$$

$$C^+(\mu) := \frac{\pi G}{9|\mu_o|^3} | |\mu + 3\mu_o|^{3/2} - |\mu + \mu_o|^{3/2} |, \quad C^-(\mu) := C^+(\mu - 4\mu_o). \quad (1.2.26)$$

Equation (1.2.24) has been derived formally by making use of states which belong to $\mathcal{F} := \mathcal{F}_g \otimes \mathcal{F}_\phi$, where \mathcal{F}_g and \mathcal{F}_ϕ are dense subspaces of the kinematical Hilbert spaces \mathcal{H}_{kin}^g and \mathcal{H}_{kin}^ϕ , respectively. The space \mathcal{F} provides an arena for the derivation of quantum dynamics. However, the physical states are expected to be in \mathcal{F}^* , the algebraic dual of \mathcal{F} (see, e.g. [14, 21] and references therein). It is known that $\mathcal{F} \subset \mathcal{H}_{kin} \subset \mathcal{F}^*$. Physical states are expected to have the form $\langle \Psi | := \sum_\mu \psi(\mu, \phi) \langle \mu |$, where $\langle \mu |$ is the eigenbras of \hat{p} . One may give the structure of the Hilbert space to some subspace of \mathcal{F}^* (constructed from solutions to (1.2.24)) by making use of the group averaging method [34, 35] and obtain this way the physical Hilbert space \mathcal{H}_{phys} .

The argument ϕ in $\psi(\mu, \phi)$ is interpreted as an evolution parameter, μ is regarded as the physical degree of freedom. Let us examine the role of the parameter μ_o

in (1.2.24). First of all, its presence causes that (1.2.24) is a difference-differential equation so its solution should be examined on a lattice. It is clear that some special role must be played by $\mu_o = 0$ as the coefficient functions of the equation, defined by (1.2.25) and (1.2.26), are singular there. One can verify [21] that as $\mu_o \rightarrow 0$ the equation (1.2.24) turns into the Wheeler-DeWitt equation

$$B(\mu) \frac{\partial^2}{\partial \phi^2} \psi(\mu, \phi) - \frac{16\pi G}{3} \frac{\partial}{\partial \mu} \sqrt{\mu} \frac{\partial}{\partial \mu} \psi(\mu, \phi) = 0, \quad \text{with } B(\mu) := \left| \frac{4\pi\gamma G\hbar}{3} \mu \right|^{-3/2}. \quad (1.2.27)$$

Equation (1.2.24) is not specially sensitive to any other value of μ_o . Thus, the determination of the numerical value of this parameter by making use of the mathematical structure of (1.2.24) seems to be impossible.

1.2.3 Minimum length problem

The singularity resolution offered by LQC, in the context of flat FRW universe, is a striking result. Let us look at the key ingredients of the construction of LQC which are responsible for this long awaited result:

Discussing the mathematical structure of the constraint equation we have found that μ_o must be a non-zero if we wish to deal with the regular (1.2.24) instead of the singular (1.2.27). However, the numerical value of μ_o cannot be determined from the equation (1.2.24). It plays the role of a free parameter if it is not specified.

The parameter μ_o enters the formalism due to the representation of the curvature of the connection F_{ab}^k via the holonomy around a loop (1.2.3). The smaller the loop the better approximation we have. The size of the loop, μ_o , determines the quantum operator corresponding to the modified gravitational part of the Hamiltonian (1.2.21). One may determine μ_o by making use of an area of the loop (used in fact as a technical

tool). Thus, the spectrum of the quantum operator corresponding to an area operator, \widehat{Ar} , seems to be a suitable source of information on the possible values of μ_o . Previous section shows explicitly that the construction of the quantum level is heavily based on the kinematical ingredients of the formalism. Thus, it is natural to explore the kinematical \widehat{Ar} of LQC. However, its spectrum (1.2.22) is continuous so it is useless for the determination of μ_o . On the other hand, the spectrum of kinematical \widehat{Ar} of LQG is discrete [32, 33]. Thus, it was tempting to use such a spectrum to fix μ_o postulating that the minimum quantum of area defines the minimum area of the loop defining (1.2.21). This way μ_o has been fixed.

The physical justification, however, for such procedure is doubtful because LQC is not the cosmological sector of LQG. Therefore, Eq. (1.2.21) includes an insertion by hand of specific properties of the spectrum of \widehat{Ar} from LQG into LQC [36]. After all, the area gap of the spectrum of \widehat{Ar} of LQG is not a fundamental constant (like the speed of light, Planck's constant, Newton's constant) so its use in the context of LQC has poor physical justification.

1.2.4 Summary

First of all we have shown that the introduction of the quantum of an area from LQG into LQC at kinematical level is only an assumption. As a consequence, the energy scale of the Big Bounce described by λ parameter is in fact unknown. It is so because λ is a free parameter of LQC.

1.3 Formalism of nonstandard LQC

Now we will present an alternative method of canonical quantization of cosmological models of GR, which makes use of loop geometry [37, 38, 39]. We believe that the nonstandard LQC may be related with the reduced phase space quantization of Loop Quantum Gravity [40]. What is the motivation for developing an alternative formalism? First of all, agreement of results obtained with both methods would be a sort of proof that the procedure of quantization is correct. Of course the final test is always an agreement with observational data when they become available. Another reason to develop an alternative approach is improving our understanding of some conceptual issues like identification of physical observables or quantum evolution of a system with the Hamiltonian constraint.

1.3.1 Main idea

In the nonstandard LQC [37, 38] one first solves the constraint (the constraints) at the classical level to identify the physical phase space (i.e. the space of Dirac's observables). Secondly, in that space one finds the elementary observables and their algebra. These elementary observables are used as “building blocks” for the compound observables, like the energy density or the volume of the universe, so they have deep physical meaning. The compound observables are thus defined on the physical phase space too. Thus, their properties may be confronted in future with the data of observational cosmology. The compound observables depend on the elementary ones and an evolution parameter¹, so for fixed moments of time they are functions only of elementary observables. Next step is a quantization. By this term we mean finding a

¹which is value of the scalar field ϕ

self-adjoint representation of the algebra of the elementary observables and solution to the eigenvalue problem for operators corresponding to the compound observables [38].

The difference of understanding the term “quantization” is a source of another difference between these two LQC methods. In nonstandard formalism, approximation of the curvature of connection by a holonomy along a loop of finite size (modification of Hamiltonian by loops) is done entirely at the classical level. Our approach is different from the so-called polymerization method practisized by users of standard LQC and treated as an effective quantum theory (see, e.g. [41]), where the modification in the Hamiltonian: $\beta \rightarrow \sin(\lambda\beta)/\lambda$ finishes the procedure of quantization. It means that in our method resolution of the singularities happens at the classical level due to loop modification of Hamiltonian. This modification is parameterized by a continuous parameter λ . There is no specific choice of λ , so we can say that λ is a free parameter. Details on theoretical ways of finding the value of λ can be found in conclusions of this Thesis.

There is also another important issue. Why should we quantize a cosmological model which is free from the cosmological singularity? We have at least three reasons: (i) to make comparison with the standard LQC results, we must have a quantum model; (ii) the parameter λ specifying the modification is a free parameter in non-standard LQC. As the result, the critical density of matter at the bounce becomes unspecified as it depends on λ . Since it may become arbitrarily big for small enough λ , the system may enter an arbitrarily small length scale, where quantum effects cannot be ignored [37]; (iii) making predictions of our model for quantum cosmic data may be used to fix the free parameter λ , after such data become available.

1.3.2 Comparison of both LQC methods

Shortly, one can write:

the standard LQC = first quantize, then impose constraints = Dirac's method;

the nonstandard LQC = first solve constraints, then quantize = reduced phase space quantization.

The most important advantage of the nonstandard LQC is that the spectra of the operators are directly obtained on physical Hilbert space. In the case of the standard LQC, one firstly obtains results on the kinematical Hilbert space. The physical states are obtained using kernels of quantum constraints operators. Applying group averaging methods leads to physical spectra of observables. Thus our nonstandard method is simpler and more efficient than the standard one.

Another important feature of nonstandard LQC is that this method is fully controlled analytically as it does not require any numerical work, at least in FRW and Bianchi I cases, in contrast to the standard LQC results.

In the nonstandard LQC an evolution parameter ϕ stays classical during the quantization. This happens because ϕ does not belong to the physical phase space. In the standard LQC ϕ is a phase space variable and should be quantized. This is crucial because ϕ being a quantum variable may fluctuate, which may make an interpretation of ϕ problematic.

1.4 Application of nonstandard LQC to FRW

In this chapter we consider, as an application of our method, the simplest cosmological model, namely FRW model with $k = 0$ and with free massless scalar field ϕ in space

with topology \mathbb{R}^3 .

1.4.1 Hamiltonian

In what follows we use the “improved” scheme $\bar{\mu} = \sqrt{\frac{1}{|p|}} \lambda$ [22]. Using it and taking (1.2.5) we calculate (1.2.8) and get the modified total Hamiltonian $H_g^{(\lambda)}$ corresponding to (1.2.9) in the form

$$H^{(\lambda)}/N = -\frac{3}{8\pi G\gamma^2} \frac{\sin^2(\lambda\beta)}{\lambda^2} v + \frac{p_\phi^2}{2v}, \quad (1.4.1)$$

where

$$\beta := \frac{c}{|p|^{1/2}}, \quad v := |p|^{3/2} \quad (1.4.2)$$

are the canonical variables proposed in [22]. The variable $\beta = \gamma\dot{a}/a$ so it corresponds to the Hubble parameter \dot{a}/a , whereas $v^{1/3} = a$ is proportional to the scale factor a .

The complete Poisson bracket for the canonical variables (β, v, ϕ, p_ϕ) is defined to be

$$\{\cdot, \cdot\} := 4\pi G\gamma \left[\frac{\partial \cdot}{\partial \beta} \frac{\partial \cdot}{\partial v} - \frac{\partial \cdot}{\partial v} \frac{\partial \cdot}{\partial \beta} \right] + \frac{\partial \cdot}{\partial \phi} \frac{\partial \cdot}{\partial p_\phi} - \frac{\partial \cdot}{\partial p_\phi} \frac{\partial \cdot}{\partial \phi}. \quad (1.4.3)$$

The dynamics of a canonical variable ξ is defined by

$$\dot{\xi} := \{\xi, H^{(\lambda)}\}, \quad \xi \in \{\beta, v, \phi, p_\phi\}, \quad (1.4.4)$$

where $\dot{\xi} := d\xi/d\tau$, and where τ is an evolution parameter. The dynamics in the physical phase space, $\mathcal{F}_{phys}^{(\lambda)}$, is defined by solutions to (1.4.4) satisfying the condition $H^{(\lambda)} \approx 0$. The solutions of (1.4.4) ignoring the constraint $H^{(\lambda)} \approx 0$ are in the kinematical phase space, $\mathcal{F}_{kin}^{(\lambda)}$.

1.4.2 Classical dynamics

Equation (1.4.1) can be rewritten as

$$H^{(\lambda)} = N H_0^{(\lambda)} \tilde{H}^{(\lambda)} \approx 0, \quad (1.4.5)$$

where

$$H_0^{(\lambda)} := \frac{3}{8\pi G \gamma^2 v} \left(\kappa \gamma |p_\phi| + v \frac{|\sin(\lambda \beta)|}{\lambda} \right), \quad \tilde{H}^{(\lambda)} := \kappa \gamma |p_\phi| - v \frac{|\sin(\lambda \beta)|}{\lambda}, \quad (1.4.6)$$

where $\kappa^2 \equiv 4\pi G/3$.

It is clear that $H_0^{(\lambda)} = 0$ only in the case when $p_\phi = 0 = \sin(\lambda \beta)$. Such case, due to (1.4.7)-(1.4.11), implies no dynamics.

Choosing the gauge $N := 1/H_0^{(\lambda)}$ (which simplifies the calculations) we get

$$\dot{p}_\phi = 0, \quad (1.4.7)$$

$$\dot{\beta} = -4\pi G \gamma \frac{|\sin(\lambda \beta)|}{\lambda}, \quad (1.4.8)$$

$$\dot{\phi} = \kappa \gamma \operatorname{sgn}(p_\phi), \quad (1.4.9)$$

$$\dot{v} = 4\pi G \gamma v \cos(\lambda \beta) \operatorname{sgn}(\sin(\lambda \beta)), \quad (1.4.10)$$

$$\tilde{H}^{(\lambda)} = 0. \quad (1.4.11)$$

Combining (1.4.9) with (1.4.10) gives

$$\frac{\dot{v}}{\dot{\phi}} = 3\kappa v \cos(\lambda \beta) \operatorname{sgn}(\sin(\lambda \beta)) \operatorname{sgn}(p_\phi). \quad (1.4.12)$$

Rewriting (1.4.12) (and using $\dot{v}/\dot{\phi} = dv/d\phi$) gives

$$\frac{\operatorname{sgn}(\sin(\lambda \beta))}{\cos(\lambda \beta)} \frac{dv}{v} = 3\kappa \operatorname{sgn}(p_\phi) d\phi \quad (1.4.13)$$

Making use of the identity $\sin^2(\lambda \beta) + \cos^2(\lambda \beta) = 1$ and (1.4.11) gives

$$|\cos(\lambda \beta)| = \sqrt{1 - \left(\frac{\kappa \gamma p_\phi \lambda}{v} \right)^2} \quad (1.4.14)$$

Combining (1.4.13) with (1.4.14), for $\beta \in]0, \pi/2\lambda[$, leads to

$$\frac{dv}{\sqrt{v^2 - (\kappa\gamma\lambda p_\phi)^2}} = 3\kappa \operatorname{sgn}(p_\phi) d\phi. \quad (1.4.15)$$

Since p_ϕ is just a constant (due to (1.4.7)) we can easily integrate (1.4.15) and get

$$\ln \left| v + \sqrt{v^2 - (\kappa\gamma\lambda p_\phi)^2} \right| = 3\kappa \operatorname{sgn}(p_\phi)(\phi - \phi_0). \quad (1.4.16)$$

Rewriting (1.4.16) leads to

$$2v = \exp(3\kappa \operatorname{sgn}(p_\phi)(\phi - \phi_0)) + (\kappa\gamma|p_\phi|\lambda)^2 \cdot \exp(-3\kappa \operatorname{sgn}(p_\phi)(\phi - \phi_0)). \quad (1.4.17)$$

The solution for the variable β may be easily determined from (1.4.11) rewritten as

$$\kappa\gamma|p_\phi| = v \frac{|\sin(\lambda\beta)|}{\lambda} \quad (1.4.18)$$

Finally we get

$$\sin(\lambda\beta) = \frac{2\kappa\gamma\lambda|p_\phi|}{\exp(3\kappa \operatorname{sgn}(p_\phi)(\phi - \phi_0)) + (\kappa\gamma\lambda p_\phi)^2 \exp(-3\kappa \operatorname{sgn}(p_\phi)(\phi - \phi_0))} \quad (1.4.19)$$

where the domain of the variable β has been extended to the interval $]0, \pi/\lambda[$.

Equations (1.4.17) and (1.4.19) present the dependence of the canonical variables v and β on the evolution parameter ϕ , which is a monotonic function due to (1.4.9).

1.4.3 Observables

Elementary observables and their algebra

A function, \mathcal{O} , defined on phase space is a Dirac observable if

$$\{\mathcal{O}, H^{(\lambda)}\} \approx 0. \quad (1.4.20)$$

Since we have

$$\{\mathcal{O}, H^{(\lambda)}\} = \{\mathcal{O}, NH_0^{(\lambda)}\tilde{H}^{(\lambda)}\} = NH_0^{(\lambda)}\{\mathcal{O}, \tilde{H}^{(\lambda)}\} + \{\mathcal{O}, NH_0^{(\lambda)}\}\tilde{H}^{(\lambda)}, \quad (1.4.21)$$

it is clear that on the constraint surface, $\tilde{H}^{(\lambda)} = 0$, the Dirac observable satisfies (independently on the choice of N) a much simpler equation

$$\{\mathcal{O}, \tilde{H}^{(\lambda)}\} \approx 0. \quad (1.4.22)$$

Using the gauge $N := 1/H_0^{(\lambda)}$ and solve (1.4.20) in the whole phase space, i.e. we solve the equation

$$\frac{\sin(\lambda\beta)}{\lambda} \frac{\partial \mathcal{O}}{\partial \beta} - v \cos(\lambda\beta) \frac{\partial \mathcal{O}}{\partial v} - \frac{\kappa \operatorname{sgn}(p_\phi)}{4\pi G} \frac{\partial \mathcal{O}}{\partial \phi} = 0. \quad (1.4.23)$$

A function $\mathcal{O} = \mathcal{O}(\mathcal{O}_1, \dots, \mathcal{O}_k)$ satisfies (1.4.23) if

$$\{\mathcal{O}_1, \tilde{H}^{(\lambda)}\} = 0 = \{\mathcal{O}_2, \tilde{H}^{(\lambda)}\} = \dots = \{\mathcal{O}_k, \tilde{H}^{(\lambda)}\}, \quad (1.4.24)$$

where $k+1$ is the dimension of the kinematical phase space. It is so because one has

$$\{\mathcal{O}, \tilde{H}^{(\lambda)}\} = \frac{\partial \mathcal{O}}{\partial \mathcal{O}_1} \{\mathcal{O}_1, \tilde{H}^{(\lambda)}\} + \dots + \frac{\partial \mathcal{O}}{\partial \mathcal{O}_k} \{\mathcal{O}_k, \tilde{H}^{(\lambda)}\}. \quad (1.4.25)$$

In what follows we consider only elementary observables. The set of such observables, \mathcal{E} , is defined by the requirements: (i) each element of \mathcal{E} is a solution to (1.4.23), (ii) elements of \mathcal{E} are functionally independent on the constraint surface, $\tilde{H}^{(\lambda)} = 0$, (iii) elements of \mathcal{E} satisfy a Lie algebra, and (iv) two sets of observables satisfying two algebras are considered to be the same if these algebras are isomorphic.

In our case $k = 3$ and solutions to (1.4.23) are found to be

$$\mathcal{O}_1 := p_\phi, \quad \mathcal{O}_2 := \phi - \frac{s}{3\kappa} \operatorname{arth}(\cos(\lambda\beta)), \quad \mathcal{O}_3 := s v \frac{\sin(\lambda\beta)}{\lambda}, \quad (1.4.26)$$

where $s := \text{sgn}(p_\phi)$. One may verify that the observables satisfy the Lie algebra

$$\{\mathcal{O}_2, \mathcal{O}_1\} = 1, \quad \{\mathcal{O}_1, \mathcal{O}_3\} = 0, \quad \{\mathcal{O}_2, \mathcal{O}_3\} = \gamma\kappa. \quad (1.4.27)$$

Because of the constraint $\tilde{H}^{(\lambda)} = 0$ (see (1.4.18)), we have

$$\mathcal{O}_3 = \gamma\kappa \mathcal{O}_1. \quad (1.4.28)$$

Thus, we have only two elementary Dirac observables which may be used to parameterize the physical phase space $\mathcal{F}_{phys}^{(\lambda)}$. To identify the Poisson bracket in $\mathcal{F}_{phys}^{(\lambda)}$ consistent with the Poisson bracket (1.4.3) defined in $\mathcal{F}_{kin}^{(\lambda)}$, we find a symplectic twoform corresponding to (1.4.3). It reads

$$\omega = \frac{1}{4\pi G\gamma} d\beta \wedge dv + d\phi \wedge dp_\phi. \quad (1.4.29)$$

The twoform ω is degenerate on $\mathcal{F}_{phys}^{(\lambda)}$ due to the constraint $\tilde{H}^{(\lambda)} = 0$. Making use of the explicit form of this constraint (1.4.18) and the functional form of \mathcal{O}_1 and \mathcal{O}_2 , leads to the symplectic form Ω on $\mathcal{F}_{phys}^{(\lambda)}$. Direct calculations give

$$\Omega := \omega_{|\tilde{H}^{(\lambda)}=0} = d\mathcal{O}_2 \wedge d\mathcal{O}_1, \quad (1.4.30)$$

where $\omega_{|\tilde{H}^{(\lambda)}=0}$ denotes the reduction of ω to the constraint surface. The Poisson bracket corresponding to (1.4.30) reads

$$\{\cdot, \cdot\} := \frac{\partial \cdot}{\partial \mathcal{O}_2} \frac{\partial \cdot}{\partial \mathcal{O}_1} - \frac{\partial \cdot}{\partial \mathcal{O}_1} \frac{\partial \cdot}{\partial \mathcal{O}_2} \quad (1.4.31)$$

so the algebra satisfied by \mathcal{O}_1 and \mathcal{O}_2 has a simple form given by

$$\{\mathcal{O}_2, \mathcal{O}_1\} = 1. \quad (1.4.32)$$

Our kinematical phase space, $\mathcal{F}_{kin}^{(\lambda)}$, is four dimensional. In relative dynamics one variable is used to parameterize three others. Since the constraint relates the variables, we have only two independent variables. This is the reason we have only two elementary physical observables parameterizing $\mathcal{F}_{phys}^{(\lambda)}$.

Functions on phase space

Now we discuss the functions on the constraint surface that may describe singularity aspects of our cosmological model. Considered functions are functions of elementary observables and evolution parameter ϕ , so they are not observables. They become observables for fixed ϕ .

An interesting function is energy density ρ of the scalar field ϕ

$$\rho(\lambda, \phi) = \frac{1}{2} \frac{p_\phi^2}{v^2}. \quad (1.4.33)$$

In terms of elementary observables we have

$$p_\phi = \mathcal{O}_1, \quad v = \kappa\gamma\lambda |\mathcal{O}_1| \cosh(3\kappa(\phi - \mathcal{O}_2)) \quad (1.4.34)$$

which means that

$$\rho(\lambda, \phi) = \frac{1}{2} \frac{1}{(\kappa\gamma\lambda)^2 \cosh^2 3\kappa(\phi - \mathcal{O}_2)}. \quad (1.4.35)$$

For fixed p_ϕ the density ρ takes its maximum value at the minimum value of v .

Rewriting (1.4.17) in the form

$$\frac{v}{\Delta} = \cosh(3\kappa s(\phi - \phi_0) - \ln \Delta), \quad \text{where} \quad \Delta := \kappa\gamma\lambda |p_\phi|, \quad (1.4.36)$$

we can see that $\cosh(\cdot)$ takes minimum value equal to one at $3\kappa s(\phi - \phi_0) = \ln \Delta$.

Thus, the maximum value of the density, ρ_{\max} , corresponds to $v = \Delta$ and reads

$$\rho_{\max} = \frac{1}{2\kappa^2\gamma^2} \frac{1}{\lambda^2}. \quad (1.4.37)$$

which means that the Big Bounce occurs at the classical level due to modification classical Hamiltonian by loops. We can determine ρ_{\max} if we know λ , but as we now λ is a free parameter of the formalism.

Another interesting observable is a volume. In terms of observables it reads [37]

$$v(\lambda, \phi) = \kappa\gamma\lambda |\mathcal{O}_1| \cosh 3\kappa(\phi - \mathcal{O}_2). \quad (1.4.38)$$

Looking at the equations written above one can see that ρ and V depend explicitly on observables \mathcal{O}_1 and \mathcal{O}_2 and evolution parameter ϕ so they are observables for fixed value of ϕ .

1.4.4 Quantization

As we remember, apart from resolving the singularity there are some important reasons to continue the procedure of the quantization.

Representation of elementary observables

For the classical algebra (1.4.32) two representations are used

$$\mathcal{O}_1 \longrightarrow \widehat{\mathcal{O}}_1 f(x) := -i\hbar \partial_x f(x), \quad \mathcal{O}_2 \longrightarrow \widehat{\mathcal{O}}_2 f(x) := \widehat{x}f(x) := xf(x), \quad (1.4.39)$$

which leads to $[\widehat{\mathcal{O}}_1, \widehat{\mathcal{O}}_2] = -i\hbar \mathbb{I}$, and

$$\mathcal{O}_1 \longrightarrow \widehat{\mathcal{O}}_1 f(x) := \widehat{x}f(x) := xf(x), \quad \mathcal{O}_2 \longrightarrow \widehat{\mathcal{O}}_2 f(x) := -i\hbar \partial_x f(x), \quad (1.4.40)$$

which leads to $[\widehat{\mathcal{O}}_1, \widehat{\mathcal{O}}_2] = i\hbar \mathbb{I}$, where $x \in \mathbb{R}$.

Due to the Stone–von Neumann theorem all self-adjoint representations of the algebra (1.4.32) are unitarily equivalent to the representation (1.4.39) or (1.4.40) defined on a suitable dense subspace of $L^2(\mathbb{R})$. In that sense the choice of representation is unique.

Energy density operator

The representation (1.4.40) is essentially self-adjoint on the dense subspace D of the Hilbert space $L^2[-r, r]$, where $r \in \mathbb{R}_+$, defined to be

$$D := \{f \in C^\infty[-r, r] \mid f^{(n)}(-r) = f^{(n)}(r), n \in \{0\} \cup \mathbb{N}\}, \quad (1.4.41)$$

where $f^{(n)} := d^n f / dx^n$.

The eigenvalue problem, $\hat{\mathcal{O}}_2 f_p = p f_p$, has the solution

$$f_p(x) = (2r)^{-1/2} \exp(ixp/\hbar), \quad p(k) := 2\pi\hbar k/r, \quad k \in \mathbb{Z}. \quad (1.4.42)$$

The spacing of neighboring eigenvalues \square is defined by

$$\square := p(k+1) - p(k) = 2\pi\hbar/r \quad (1.4.43)$$

Making r sufficiently large \square can be made as small as desired, which means that the spectrum of $\hat{\mathcal{O}}_2$ is continuous.

In the representation (1.4.40) the energy density operator reads

$$\hat{\rho} := \frac{1}{2} \frac{1}{(\kappa\gamma\lambda)^2 \cosh^2 3\kappa(\phi + i\hbar\partial_x)}. \quad (1.4.44)$$

Since $\hat{\mathcal{O}}_2$ is essentially self-adjoint on $\mathcal{F}_r := \{f_{p(k)}\}_{k \in \mathbb{Z}}$, we may apply the spectral theorem to get $\hat{\rho} f_p = \rho(\phi, \lambda, p) f_p$ where

$$\rho(\phi, \lambda, p) := \frac{1}{2} \frac{1}{(\kappa\gamma\lambda)^2 \cosh^2 3\kappa(\phi - p)}, \quad (1.4.45)$$

and where $\rho(\phi, \lambda, p)$ is the eigenvalue corresponding to the eigenvector f_p .

It is clear from our results that classical (1.4.33) and quantum (1.4.45) expressions for the energy density coincide. One may verify that the maximum density $\rho_{max}(\lambda) = \frac{1}{2} \frac{1}{(\kappa\gamma\lambda)^2}$.

Starting from the other representation we would get the quantum model of the energy density presented in [42], which is equivalent this present one.

Volume operator

To define the quantum operator corresponding to v , we introduce w defined by

$$w := \kappa\gamma\lambda \mathcal{O}_1 \cosh 3\kappa(\phi - \mathcal{O}_2). \quad (1.4.46)$$

Since $v = |w|$ it is clear that quantization of v reduces to the quantization of w . The latter may be done in a standard way as follows

$$\hat{w} f(x) := \kappa\gamma\lambda \frac{1}{2} \left(\hat{\mathcal{O}}_1 \cosh 3\kappa(\phi - \hat{\mathcal{O}}_2) + \cosh 3\kappa(\phi - \hat{\mathcal{O}}_2) \hat{\mathcal{O}}_1 \right) f(x), \quad (1.4.47)$$

where $f \in L^2(\mathbb{R})$.

For the elementary observables \mathcal{O}_1 and \mathcal{O}_2 we use the representation (1.4.39). An explicit form of the operator \hat{w} reads

$$\hat{w} f(x) = i \frac{\kappa\gamma\lambda\hbar}{2} \left(2 \cosh 3\kappa(\phi - x) \frac{d}{dx} - 3\kappa \sinh 3\kappa(\phi - x) \right) f(x). \quad (1.4.48)$$

To simplify our considerations we take f in the form

$$f(x) := A e^{ih(x)} \cosh^{-1/2} 3\kappa(\phi - x), \quad (1.4.49)$$

where h is a real-valued function and $A \in \mathbb{R}$.

Eigenvalue problem

Considering the eigenvalue problem for the operator \hat{w} in the set of functions of the form (1.4.49). We get

$$\hat{w} f(x) = -\kappa\gamma\lambda\hbar \cosh 3\kappa(\phi - x) \frac{dh(x)}{dx} f(x) =: b f(x), \quad (1.4.50)$$

where $b \in \mathbb{R}$ is the eigenvalue of \hat{w} .

A general form of h satisfying (1.4.50) is given by

$$h(x) = \frac{2b}{3\kappa^2\gamma\lambda\hbar} \arctan e^{3\kappa(\phi-x)}, \quad (1.4.51)$$

which means that a normalized f_b satisfying (1.4.50) reads

$$f_b(x) := \frac{\sqrt{\frac{3\kappa}{\pi}} \exp\left(i\frac{2b}{3\kappa^2\gamma\lambda\hbar} \arctan e^{3\kappa(\phi-x)}\right)}{\cosh^{\frac{1}{2}} 3\kappa(\phi-x)}. \quad (1.4.52)$$

Orthogonality

Using (1.4.52) we get

$$\langle f_b | f_a \rangle = \frac{3\kappa}{\pi} \int_{-\infty}^{\infty} \frac{\exp\left(i\frac{2(a-b)}{3\kappa^2\gamma\lambda\hbar} \arctan e^{3\kappa(\phi-x)}\right)}{\cosh 3\kappa(\phi-x)} dx. \quad (1.4.53)$$

The substitution $\tan z = e^{3\kappa(\phi-x)}$ leads to

$$\langle f_b | f_a \rangle = \frac{2}{\pi} \int_0^{\frac{\pi}{2}} \exp\left(i\frac{2(a-b)}{3\kappa^2\gamma\lambda\hbar} z\right) dz = -i \frac{3\kappa^2\gamma\lambda\hbar}{\pi(a-b)} \exp\left(i\frac{2(a-b)}{3\kappa^2\gamma\lambda\hbar} z\right) \Big|_0^{\frac{\pi}{2}}. \quad (1.4.54)$$

One may verify that $\langle f_b | f_a \rangle = 0$ iff

$$a - b = 6\kappa^2\gamma\lambda\hbar m = 8\pi G\gamma\lambda\hbar m, \quad m \in \mathbb{Z}. \quad (1.4.55)$$

Thus, the set $\mathcal{F}_b := \{ f_a \mid a = b + 8\pi G\gamma\lambda\hbar m; m \in \mathbb{Z}; b \in \mathbb{R} \}$ is orthonormal. Each subspace $\mathcal{F}_b \subset L^2(\mathbb{R})$ spans a pre-Hilbert space. The completion of each $\text{span } \mathcal{F}_b, \forall b \in \mathbb{R}$, gives $L^2(\mathbb{R})$ in the norm of $L^2(\mathbb{R})$.

Self-adjointness

The operator \hat{w} is symmetric on \mathcal{F}_b for any $b \in \mathbb{R}$ due to $\langle f_b | \hat{w} f_a \rangle - \langle \hat{w} f_b | f_a \rangle = (a - b) \langle f_b | f_a \rangle$ because $\langle f_b | f_a \rangle = 0$ for $a \neq b$.

To examine the self-adjointness of the unbounded operator \hat{w} , we first identify the deficiency subspaces of this operator \mathcal{K}_{\pm} [43, 44]

$$\mathcal{K}_{\pm} := \{g_{\pm} \in D_b(\hat{w}^*) \mid \langle g_{\pm} | (\hat{w} \pm i\mathbb{I}) f_a \rangle = 0, \forall f_a \in D_b(\hat{w})\}, \quad (1.4.56)$$

where $D_b(\hat{w}) := \text{span } \mathcal{F}_b$, and $D_b(\hat{w}^*) := \{f \in L^2(\mathbb{R}) : \exists! f^* \langle f^* | g \rangle = \langle f | \hat{w}g \rangle, \forall g \in D_b(\hat{w})\}$.

For each $f_a \in D_b(\hat{w}) \subset L^2(\mathbb{R})$ we have

$$0 = \langle g_{\pm} | (\hat{w} \pm i\mathbb{I}) f_a \rangle = (a \pm i) \int_{-\infty}^{\infty} dx \overline{g_{\pm}(x)} f_a(x) \implies g_+ = 0 = g_- \quad (1.4.57)$$

Thus, the deficiency indices $n_{\pm} := \dim[\mathcal{K}_{\pm}]$ of \hat{w} satisfy the relation: $n_+ = 0 = n_-$. This proves essential self-adjointness of \hat{w} on $D_b(\hat{w})$.

Spectrum

Due to the spectral theorem on self-adjoint operators [43, 44], we may quantize the volume as follows

$$v = |w| \longrightarrow \hat{v} f_a := |a| f_a. \quad (1.4.58)$$

A common feature of all \mathcal{F}_b is the existence of the minimum gap $\Delta := 8\pi G\gamma\hbar\lambda$ defining a quantum of the volume. Let us discuss this issue in more detail. Denoting the minimum eigenvalue of \hat{v} by v_{min} , one can verify that $v_{min} = \min\{b, \Delta - b\}$, where $b \in [0, \Delta[$. The spectrum consists of the union of $\{v_{min} + n\Delta\}$ and $\{-v_{min} + (n+1)\Delta\}$, where $n = 0, 1, \dots$. There are only two cases when these two subsets are identical, namely when $v_{min} = 0$ or $v_{min} = \Delta/2$, for which the minimum gap Δ is a constant gap between any two adjacent levels of the spectrum. Otherwise, the gap equals either $\Delta - 2v_{min}$ or $2v_{min}$, and the minimum gap is the smaller one. One can verify that the case of any $b \in \mathbb{R}$ reduces to the above case.

There is no quantum of the volume in the limit $\lambda \rightarrow 0$, corresponding to the classical FRW model without the loop geometry modification.

It results from (1.4.55) that for $b = 0$ and $m = 0$ the minimum eigenvalue of \hat{v} equals zero. This special case corresponds to the classical situation when $v = 0$,

which due to (1.4.1) means that $p_\phi = 0$ (no classical dynamics). Thus, we have a direct correspondence between classical and quantum levels corresponding to this very special state. All other states describe bouncing dynamics.

Evolution

It is clear that the relation between eigenvectors corresponding to the same eigenvalue for different values of the parameter ϕ reads $f_a^{\phi+\psi} = e^{\psi\partial_\phi} f_a^\phi = e^{-i\frac{\psi}{\hbar}\hat{O}_1} f_a^\phi$.

One may verify that

$$\hat{w}(\phi + \psi) = \cosh(3\kappa\psi)\hat{w}(\phi) + \frac{\sinh(3\kappa\psi)}{3\kappa}\partial_\phi\hat{w}(\phi), \quad (1.4.59)$$

thus

$$\begin{aligned} \langle f_b^\phi | \hat{w}(\phi + \psi) f_a^\phi \rangle &= \langle f_b^\phi | \hat{w}(\phi) f_a^\phi \rangle \cosh(3\kappa\psi) + \frac{\sinh(3\kappa\psi)}{3\kappa} \langle f_b^\phi | \partial_\phi \hat{w}(\phi) f_a^\phi \rangle \\ &= a \cosh(3\kappa\psi) \delta_{ab} + (b - a) \frac{\sinh(3\kappa\psi)}{3\kappa} \langle f_b^\phi | \partial_x f_a^\phi \rangle. \end{aligned} \quad (1.4.60)$$

An evolution of the expectation value of the operator \hat{w} is found to be

$$\langle f(\phi) | \hat{w}(\phi + \psi) f(\phi) \rangle = A \cosh 3\kappa(\psi + B), \quad (1.4.61)$$

where $f := \sum \alpha_a f_a$, $f_a \in \mathcal{F}_b$.

One may verify that

$$A = \text{sgn}(X)\sqrt{X^2 - Y^2}, \quad B = \frac{1}{6\kappa} \ln \frac{X + Y}{X - Y}, \quad (1.4.62)$$

where

$$X := \sum_a |\alpha_a|^2 a, \quad Y := \sum_{a, m} \frac{\bar{\alpha}_b \alpha_a - \bar{\alpha}_a \alpha_b}{i\pi} \frac{m(2a + 6m\kappa^2\gamma\hbar\lambda)}{(2m-1)(2m+1)}, \quad (1.4.63)$$

and where $b = a + 6\kappa^2\gamma\lambda\hbar$, $b \in \mathbb{R}$, $m \in \mathbb{Z}$, and $|X| > |Y|$.

One can see that the evolution of the expectation value of the operator \hat{w} coincides with the classical expression (1.4.46).

1.4.5 Summary

The resolution of the cosmological singularity is due to the loop modification of the Hamiltonian already at the classical level. This modification is parameterized by a continuous parameter λ , whose value is so far unknown. Each value of that parameter specifies quantum of the volume and the maximum energy density of the matter (scalar field in our model).

Spectrum of the volume operator is bounded from below and discrete. Its expectation value coincides with the classical expression.

The spectrum of the energy density is bounded from below and continuous. There is a coincidence between classical and quantum expressions for the maximum energy density.

Chapter 2

Bianchi I model in terms of nonstandard LQC

From Introduction we know that the Bianchi I model of the Universe is of primary importance as it underlies, to some extent, the Belinskii-Khalatnikov-Lifshitz (BKL) scenario [11, 45, 46, 47, 48], which is believed to describe the Universe in the vicinity of the cosmological singularity. It has been examined recently within the nonstandard LQC [49, 50], and has been also studied in the context of the standard LQC [13, 19, 51, 52, 53]. Clear exposition of the singularity aspects of the Bianchi I model can be found in [41, 48].

This chapter presents analyzes of the Bianchi I model within the nonstandard LQC formalism. In what follows we consider the Bianchi I model with free massless scalar field in T^3 topology. We choose this topology, because taking \mathbb{R}^3 might lead to problems with interpretation of the spectra of the volume operator [50].

2.1 Classical level

2.1.1 Hamiltonian

The Bianchi I model with massless scalar field is described by the metric:

$$ds^2 = -N^2 dt^2 + \sum_{i=1}^3 a_i^2(t) dx_i^2, \quad (2.1.1)$$

where

$$a_i(\tau) = a_i(0) \left(\frac{\tau}{\tau_0} \right)^{k_i}, \quad d\tau = N dt, \quad \sum_{i=1}^3 k_i = 1 = \sum_{i=1}^3 k_i^2 + k_\phi^2, \quad (2.1.2)$$

and where k_ϕ describes matter field density ($k_\phi = 0$ corresponds to the Kasner model).

To make this chapter self-contained we remind that in GR the gravitational part of the classical Hamiltonian, H_g , is a linear combination of the first-class constraints

$$H_g := \int_{\Sigma} d^3x (N^i C_i + N^a C_a + NC), \quad (2.1.3)$$

where Σ is the spacelike part of spacetime $\mathbb{R} \times \Sigma$, (N^i, N^a, N) denote Lagrange multipliers, (C_i, C_a, C) are the Gauss, diffeomorphism and scalar constraint functions. In our notation ($a, b = 1, 2, 3$) are spatial and ($i, j, k = 1, 2, 3$) are internal $SU(2)$ indices. As we know the constraints must satisfy a specific algebra.

Having fixed local gauge and diffeomorphism freedom we can rewrite it for the Bianchi I model with massless scalar field [49]

$$H_g = -\gamma^{-2} \int_{\mathcal{V}} d^3x Ne^{-1} \varepsilon_{ijk} E^{aj} E^{bk} F_{ab}^i, \quad (2.1.4)$$

where γ is the Barbero-Immirzi parameter, $\mathcal{V} \subset \Sigma$ is an elementary cell, Σ is spacelike hypersurface, N denotes the lapse function, ε_{ijk} is the alternating tensor, E_i^a is a densitized vector field, $e := \sqrt{|\det E|}$, and where F_{ab}^i is the curvature of an $SU(2)$ connection A_a^i .

As we know, the resolution of the singularity, obtained within LQC, is based on rewriting the curvature F_{ab}^k in terms of holonomies around loops. The curvature F_{ab}^k may be determined by making use of the formula

$$F_{ab}^k = -2 \lim_{Ar \square_{ij} \rightarrow 0} Tr \left(\frac{h_{\square_{ij}} - 1}{Ar \square_{ij}} \right) \tau^k {}^o\omega_a^i {}^o\omega_a^j, \quad (2.1.5)$$

where

$$h_{\square_{ij}} = h_i^{(\mu_i)} h_j^{(\mu_j)} (h_i^{(\mu_i)})^{-1} (h_j^{(\mu_j)})^{-1} \quad (2.1.6)$$

is the holonomy of the gravitational connection around the square loop \square_{ij} , considered over a face of the elementary cell, each of whose sides has length $\mu_j L_j$ (and $V_o := L_1 L_2 L_3$) with respect to the flat fiducial metric ${}^oq_{ab} := \delta_{ij} {}^o\omega_a^i {}^o\omega_a^j$; the fiducial triad ${}^o e_k^a$ and cotriad ${}^o\omega_a^k$ satisfy ${}^o\omega_a^i {}^o e_j^a = \delta_j^i$; $Ar \square_{ij}$ denotes the area of the square; and $V_o = \int_{\mathcal{V}} \sqrt{{}^oq} d^3x$ is the fiducial volume of \mathcal{V} .

The holonomy in the fundamental, $j = 1/2$, representation of $SU(2)$ reads

$$h_i^{(\mu_i)} = \cos(\mu_i c_i/2) \mathbb{I} + 2 \sin(\mu_i c_i/2) \tau_i, \quad (2.1.7)$$

where $\tau_i = -i\sigma_i/2$ (σ_i are the Pauli spin matrices). The connection A_a^k and the density weighted triad E_i^a (which occurs in (2.1.11)) are determined by the conjugate variables c and p :

$$A_a^i = c_i L_i^{-1} {}^o\omega_a^i, \quad E_i^a = p_i L_j^{-1} L_k^{-1} {}^o e_i^a, \quad (2.1.8)$$

where:

$$c_i = \gamma \dot{a}_i L_i, \quad |p_i| = a_j a_k L_j L_k. \quad (2.1.9)$$

and

$$\{c_i, p_j\} = 8\pi G \gamma \delta_{ij} \quad (2.1.10)$$

Making use of (2.1.4), (2.1.5) and the so-called Thiemann identity

$$\varepsilon_{ijk} e^{-1} E^{aj} E^{bk} = \frac{\text{sgn}(p_1 p_2 p_3)}{2\pi G \gamma (\mu_1 \mu_2 \mu_3)^{1/3}} \sum_k {}^o\varepsilon^{abc} {}^o\omega_c^k \text{Tr} \left(h_k^{(\mu_k)} \{(h_k^{(\mu_k)})^{-1}, V\} \tau_i \right) \quad (2.1.11)$$

leads to H_g in the form

$$H_g = \lim_{\mu_1, \mu_2, \mu_3 \rightarrow 0} H_g^{(\mu_1 \mu_2 \mu_3)}, \quad (2.1.12)$$

where

$$H_g^{(\mu_1 \mu_2 \mu_3)} = -\frac{\text{sgn}(p_1 p_2 p_3)}{2\pi G \gamma^3 \mu_1 \mu_2 \mu_3} \sum_{ijk} N \varepsilon^{ijk} \text{Tr} \left(h_i^{(\mu_i)} h_j^{(\mu_j)} (h_i^{(\mu_i)})^{-1} (h_j^{(\mu_j)})^{-1} h_k^{(\mu_k)} \{(h_k^{(\mu_k)})^{-1}, V\} \right), \quad (2.1.13)$$

and where $V = a_1 a_2 a_3 L_1 L_2 L_3$ is the volume of the elementary cell \mathcal{V} .

The total Hamiltonian for Bianchi I universe with a massless scalar field, ϕ , reads

$$H = H_g + H_\phi \approx 0, \quad (2.1.14)$$

where H_g is defined by (2.1.12). The Hamiltonian of the scalar field is known to be: $H_\phi = N p_\phi^2 |p_1 p_2 p_3|^{-\frac{1}{2}} / 2$, where ϕ and p_ϕ are the elementary variables satisfying $\{\phi, p_\phi\} = 1$. The relation $H \approx 0$ defines the physical phase space of considered gravitational system with constraints.

Making use of (2.1.7) we calculate (2.1.13) and get the modified total Hamiltonian $H_g^{(\lambda)}$ corresponding to (2.1.14) in the form

$$H^{(\lambda)}/N = -\frac{1}{8\pi G \gamma^2} \frac{\text{sgn}(p_1 p_2 p_3)}{\mu_1 \mu_2 \mu_3} \left[\sin(c_1 \mu_1) \sin(c_2 \mu_2) \mu_3 \text{sgn}(p_3) \sqrt{\frac{|p_1 p_2|}{|p_3|}} + \text{cyclic} \right] + \frac{p_\phi^2}{2V} \quad (2.1.15)$$

where

$$\mu_i := \sqrt{\frac{1}{|p_i|}} \lambda, \quad (2.1.16)$$

and where λ is a regularization parameter. Here we wish to emphasize that (2.1.15) presents a loop modified but classical Hamiltonian.

It is known [13, 41, 52] that such a choice of μ_i leads to the dependence of the final results on the fiducial volume V_0 . In the universe with compact topology, like that considered by us, V_0 has physical sense, in contrast to a case with noncompact topology. Thus, an expected dependence of the results on V_0 would be rather meritorious than problematic.

In the gauge $N = \sqrt{|p_1 p_2 p_3|}$ the Hamiltonian modified by loop geometry reads

$$H^{(\lambda)} = -\frac{1}{8\pi G\gamma^2 \lambda^2} \left[|p_1 p_2|^{3/2} \sin(c_1 \mu_1) \sin(c_2 \mu_2) + \text{cyclic} \right] + \frac{p_\phi^2}{2}. \quad (2.1.17)$$

The Poisson bracket is defined to be

$$\{\cdot, \cdot\} := 8\pi G\gamma \sum_{k=1}^3 \left[\frac{\partial \cdot}{\partial c_k} \frac{\partial \cdot}{\partial p_k} - \frac{\partial \cdot}{\partial p_k} \frac{\partial \cdot}{\partial c_k} \right] + \frac{\partial \cdot}{\partial \phi} \frac{\partial \cdot}{\partial p_\phi} - \frac{\partial \cdot}{\partial p_\phi} \frac{\partial \cdot}{\partial \phi}, \quad (2.1.18)$$

where $(c_1, c_2, c_3, p_1, p_2, p_3, \phi, p_\phi)$ are canonical variables. The dynamics of ξ reads

$$\dot{\xi} := \{\xi, H^{(\lambda)}\}, \quad \xi \in \{c_1, c_2, c_3, p_1, p_2, p_3, \phi, p_\phi\}. \quad (2.1.19)$$

The dynamics in the physical phase space, $\mathcal{F}_{phys}^{(\lambda)}$, is defined by solutions to (2.1.19) satisfying the condition $H^{(\lambda)} \approx 0$. The solutions of (2.1.19) ignoring the constraint $H^{(\lambda)} \approx 0$ are in the kinematical phase space, $\mathcal{F}_{kin}^{(\lambda)}$.

We use the following canonical variables

$$\beta_i := \frac{c_i}{\sqrt{|p_i|}}, \quad v_i := |p_i|^{3/2}, \quad (2.1.20)$$

where $i = 1, 2, 3$. They satisfy the algebra

$$\{\beta_i, v_j\} = 12\pi G\gamma \delta_{ij}, \quad (2.1.21)$$

where the Poisson bracket reads

$$\{\cdot, \cdot\} = 12\pi G\gamma \sum_{k=1}^3 \left[\frac{\partial \cdot}{\partial \beta_k} \frac{\partial \cdot}{\partial v_k} - \frac{\partial \cdot}{\partial v_k} \frac{\partial \cdot}{\partial \beta_k} \right] + \frac{\partial \cdot}{\partial \phi} \frac{\partial \cdot}{\partial p_\phi} - \frac{\partial \cdot}{\partial p_\phi} \frac{\partial \cdot}{\partial \phi}. \quad (2.1.22)$$

The Hamiltonian in the variables (2.1.20) turns out to be

$$H^{(\lambda)} = \frac{p_\phi^2}{2} - \frac{1}{8\pi G\gamma^2} \left(\frac{\sin(\lambda\beta_1)\sin(\lambda\beta_2)}{\lambda^2} v_1 v_2 + \frac{\sin(\lambda\beta_1)\sin(\lambda\beta_3)}{\lambda^2} v_1 v_3 + \frac{\sin(\lambda\beta_2)\sin(\lambda\beta_3)}{\lambda^2} v_2 v_3 \right), \quad (2.1.23)$$

where λ parameterizes the holonomy of connection modifying the Bianchi I model.

2.1.2 Classical dynamics

The Hamilton equations of motion read

$$\dot{\beta}_i = -18\pi G \frac{\sin(\lambda\beta_i)}{\lambda} (O_j + O_k), \quad (2.1.24)$$

$$\dot{v}_i = 18\pi G v_i \cos(\lambda\beta_i) (O_j + O_k), \quad (2.1.25)$$

$$\dot{\phi} = p_\phi, \quad (2.1.26)$$

$$\dot{p}_\phi = 0, \quad (2.1.27)$$

$$H^{(\lambda)} \approx 0, \quad (2.1.28)$$

where $i, j, k = 1, 2, 3$ and $i \neq j \neq k$ and where

$$O_i := \frac{v_i \sin(\lambda\beta_i)}{12\pi G\gamma\lambda}. \quad (2.1.29)$$

Insertion of (2.1.25) into (2.1.24) gives

$$d\beta_i = -\frac{\tan(\lambda\beta_i)}{\lambda} \frac{dv_i}{v_i}, \quad (2.1.30)$$

which leads to

$$v_i \frac{\sin(\lambda\beta_i)}{\lambda} = \text{const} \quad (2.1.31)$$

Therefore, O_i are constants of motion.

Making use of (2.1.26), (2.1.25) and $\cos(\lambda\beta_i) = \sqrt{1 - \sin(\lambda\beta_i)^2}$ gives

$$\int \frac{dv_i}{\sqrt{v_i^2 - (12\pi G\gamma\lambda O_i)^2}} = 18\pi G \int \frac{(O_j + O_k)}{p_\phi} d\phi. \quad (2.1.32)$$

Integration of (2.1.32) leads to

$$\ln \left| v_i + \sqrt{v_i^2 - (12\pi G\gamma\lambda O_i)^2} \right| = \frac{18\pi G}{p_\phi} (O_j + O_k) (\phi - \phi_i^0). \quad (2.1.33)$$

Thus we have

$$\begin{aligned} 2|v_i| &= \exp \left(\frac{18\pi G}{p_\phi} (O_j + O_k) (\phi - \phi_i^0) \right) + (12\pi G\gamma\lambda O_i)^2 \times \\ &\quad \times \exp \left(- \frac{18\pi G}{p_\phi} (O_j + O_k) (\phi - \phi_i^0) \right), \end{aligned} \quad (2.1.34)$$

which may be rewritten as

$$v_i = 12\pi G\gamma\lambda |O_i| \cosh \left(\frac{18\pi G}{p_\phi} (O_j + O_k) (\phi - \phi_i^0) - \ln |12\pi G\gamma\lambda O_i| \right). \quad (2.1.35)$$

2.1.3 Elementary observables

As we know, function F defined on the phase space is a Dirac observable if it is a solution to the equation

$$\{F, H^{(\lambda)}\} \approx 0. \quad (2.1.36)$$

An explicit form of (2.1.36) is given by

$$12\pi G\gamma \sum_{i=1}^3 \left(\frac{\partial F}{\partial \beta_i} \frac{\partial H^{(\lambda)}}{\partial v_i} - \frac{\partial F}{\partial v_i} \frac{\partial H^{(\lambda)}}{\partial \beta_i} \right) + \frac{\partial F}{\partial \phi} p_\phi = 0, \quad (2.1.37)$$

which reads

$$18\pi G \sum_{i=1}^3 \left[v_i \cos(\lambda\beta_i) \frac{\partial F}{\partial v_i} - \frac{\sin(\lambda\beta_i)}{\lambda} \frac{\partial F}{\partial \beta_i} \right] \cdot (O_j + O_k) + \frac{\partial F}{\partial \phi} p_\phi = 0. \quad (2.1.38)$$

Kinematical observables

One may easily verify that O_i satisfy (2.1.38). Instead of solving (2.1.38) one may use the constants that occur in (2.1.35). This way we get

$$A_i = \ln \left| \frac{\tan\left(\frac{\lambda\beta_i}{2}\right)}{\frac{\lambda}{2}} \right| + 18\pi G \frac{(O_j + O_k)}{p_\phi} \phi \quad (2.1.39)$$

The observables (2.1.39) are called kinematical as they are not required to satisfy the constraint (2.1.28).

Dynamical observables

An explicit form of the constraint (2.1.28) in terms of O_i is given by

$$p_\phi \operatorname{sgn}(p_\phi) = 6\sqrt{\pi G} \sqrt{O_1 O_2 + O_1 O_3 + O_2 O_3}. \quad (2.1.40)$$

It results from (22), (27) and (28) that $O_1 O_2 + O_1 O_3 + O_2 O_3 \geq 0$ so (42) is well defined. Thus, the dynamical observables, A_i^{dyn} , corresponding to (2.1.39) read

$$A_i^{\text{dyn}} = \ln \left| \frac{\tan\left(\frac{\lambda\beta_i}{2}\right)}{\frac{\lambda}{2}} \right| + \frac{3\sqrt{\pi G} \operatorname{sgn}(p_\phi)(O_j + O_k)\phi}{\sqrt{O_1 O_2 + O_1 O_3 + O_2 O_3}}. \quad (2.1.41)$$

Algebra of elementary observables

One may verify that A_i^{dyn} satisfy the following Lie algebra

$$\{O_i, O_j\} = 0, \quad (2.1.42)$$

$$\{A_i^{\text{dyn}}, O_j\} = \delta_{ij}, \quad (2.1.43)$$

$$\{A_i^{\text{dyn}}, A_j^{\text{dyn}}\} = 0. \quad (2.1.44)$$

In the physical phase space the Poisson bracket is found to be

$$\{\cdot, \cdot\}_{\text{dyn}} := \sum_{i=1}^3 \left(\frac{\partial \cdot}{\partial A_i^{\text{dyn}}} \frac{\partial \cdot}{\partial O_i} - \frac{\partial \cdot}{\partial O_i} \frac{\partial \cdot}{\partial A_i^{\text{dyn}}} \right), \quad (2.1.45)$$

and the algebra reads

$$\{O_i, O_j\}_{\text{dyn}} = 0, \quad (2.1.46)$$

$$\{A_i^{\text{dyn}}, O_j\}_{\text{dyn}} = \delta_{ij}, \quad (2.1.47)$$

$$\{A_i^{\text{dyn}}, A_j^{\text{dyn}}\}_{\text{dyn}} = 0. \quad (2.1.48)$$

2.1.4 Compound observables

In what follows we consider the physical observables which characterize the singularity aspects of the Bianchi I model. It is helpful to rewrite (2.1.40) and (2.1.35) in the form

$$p_\phi^2 = 36\pi G (O_1 O_2 + O_1 O_3 + O_2 O_3), \quad (2.1.49)$$

$$v_i = 12\pi G \gamma \lambda |O_i| \cosh \left(\frac{3\sqrt{\pi G} \operatorname{sgn}(p_\phi) (O_j + O_k) \phi}{\sqrt{O_1 O_2 + O_1 O_3 + O_2 O_3}} + \ln \left(\frac{\lambda}{2} \right) - A_i^{\text{dyn}} \right). \quad (2.1.50)$$

The so-called directional energy density [41] is defined to be

$$\rho_i(\lambda, \phi) := \frac{p_\phi^2}{2 v_i^2}. \quad (2.1.51)$$

The bounce in the i -th direction occurs when ρ_i approaches its maximum [41], which happens at the minimum of v_i (p_ϕ is a constant of motion). One may easily verify that in the case when all three directions coincide, which corresponds to the FRW model, these densities turn into the energy density of the flat FRW with massless scalar field [37].

It is clear that v_i takes minimum for $\cosh(\cdot) = 1$ so we have

$$v_i^{\min} = 12\pi G \gamma \lambda O_i, \quad \rho_i^{\max} = \frac{1}{2} \left(\frac{p_\phi}{12\pi G \gamma \lambda O_i} \right)^2. \quad (2.1.52)$$

Rewriting O_i and p_ϕ in terms of k_i and k_ϕ [41]

$$O_i = \frac{2}{3} k_i K, \quad p_\phi = \sqrt{8\pi G} k_\phi K, \quad (2.1.53)$$

where K is a constant, leads to

$$\rho_i^{max} = \frac{1}{16\pi G\gamma^2\lambda^2} \left(\frac{k_\phi}{k_i} \right)^2. \quad (2.1.54)$$

We can determine ρ_i^{max} if we know λ , but as we remember λ is a free parameter of the formalism.

One may apply (2.1.54) to the Planck scale. Substituting $\lambda = l_{Pl}$ gives

$$\rho_i^{max} \simeq 0,35 \left(\frac{k_\phi}{k_i} \right)^2 \rho_{Pl}, \quad (2.1.55)$$

which demonstrates that ρ_i^{max} may fit the Planck scale depending on the ratio k_ϕ/k_i .

Another important physical observable is the volume of the Universe. From the definitions (2.1.9) and (2.1.20) we get

$$V = a_1 a_2 a_3 = (v_1 v_2 v_3)^{1/3}. \quad (2.1.56)$$

It is clear from (2.1.50), (2.1.53) and (2.1.2) that the volume is bounded from below.

2.2 Preparations to quantization

This section is devoted to some redefinitions which are helpfull to the procedure of a quantization. The quantization is required despite the fact that the singularity problem is resolved already at the classical level due to the modifications based on the loop geometry. The reasons are described above. Here we analyze the structure of the phase space, which is obviously much more complicated than in the FRW case.

2.2.1 Redefinitions

Redefinition of evolution parameter

Firstly we slightly redefine the elementary Bianchi observables used in previous sections. Now they read

$$O_i := \frac{1}{3\kappa\gamma} \frac{v_i \sin(\lambda\beta_i)}{\lambda}, \quad (2.2.1)$$

and

$$A_i := \frac{1}{3\kappa} \ln \left(\frac{\left| \tan \left(\frac{\lambda\beta_i}{2} \right) \right|}{\frac{\lambda}{2}} \right) + \frac{3}{2\sqrt{3}} \frac{\operatorname{sgn}(p_\phi)(O_j + O_k)\phi}{\sqrt{O_1O_2 + O_1O_3 + O_2O_3}}, \quad (2.2.2)$$

where $\kappa^2 := 4\pi G/3$. One may verify that the algebra of redefined observables is isomorphic to the previous one

$$\{O_i, O_j\} = 0, \quad \{A_i, O_j\} = \delta_{ij}, \quad \{A_i, A_j\} = 0. \quad (2.2.3)$$

and

$$v_i = 3\kappa\gamma\lambda|O_i| \cosh \left(\frac{3\sqrt{\pi G}(O_j + O_k)\phi}{\sqrt{O_1O_2 + O_1O_3 + O_2O_3}} - 3\kappa A_i \right). \quad (2.2.4)$$

Since the observables O_i are constants of motion in $\phi \in \mathbb{R}$, it is possible to make the following redefinition of an evolution parameter

$$\varphi := \frac{\sqrt{3}\phi}{2\sqrt{O_1O_2 + O_1O_3 + O_2O_3}} \quad (2.2.5)$$

so we have

$$v_i = 3\kappa\gamma\lambda|O_i| \cosh 3\kappa((O_j + O_k)\varphi - A_i), \quad (2.2.6)$$

which simplifies further considerations.

New elementary observables

One can make the following redefinitions

$$\mathcal{A}_i := A_i - (O_j + O_k)\varphi. \quad (2.2.7)$$

Thus, the directional volume (2.2.6) becomes

$$v_i := |w_i|, \quad w_i = 3\kappa\gamma\lambda O_i \cosh(3\kappa\mathcal{A}_i). \quad (2.2.8)$$

The algebra of observables reads

$$\{O_i, O_j\} = 0, \quad \{\mathcal{A}_i, O_j\} = \delta_{ij}, \quad \{\mathcal{A}_i, \mathcal{A}_j\} = 0, \quad (2.2.9)$$

where the Poisson bracket is defined to be

$$\{\cdot, \cdot\} := \sum_{k=1}^3 \left(\frac{\partial \cdot}{\partial \mathcal{A}_k} \frac{\partial \cdot}{\partial O_k} - \frac{\partial \cdot}{\partial O_k} \frac{\partial \cdot}{\partial \mathcal{A}_k} \right). \quad (2.2.10)$$

2.2.2 Structure of phase space

All considerations carried out in the previous section have been done under the assumption that the observables O_1 , O_2 and O_3 have no restrictions. The inspection of (2.2.2), (2.2.4) and (2.2.7) shows that the domain of definition of the elementary observables reads

$$D := \{(\mathcal{A}_k, O_k) \mid \mathcal{A}_k \in \mathbb{R}, \quad O_1 O_2 + O_1 O_3 + O_2 O_3 > 0\}, \quad (2.2.11)$$

where $k = 1, 2, 3$. The restriction $O_1 O_2 + O_1 O_3 + O_2 O_3 > 0$ is a consequence of the Hamiltonian constraint (see, [49] for more details).

In what follows we consider two cases:

1. Kasner-unlike dynamics: (a) $O_i > 0$, $O_j > 0$, $O_k > 0$, which describes all three directions expanding (b) $O_i < 0$, $O_j < 0$, $O_k < 0$, with all directions shrinking.
2. Kasner-like dynamics: (a) $O_i > 0$, $O_j > 0$, $O_k < 0$, which describes two directions expanding and one direction shrinking; (b) $O_i < 0$, $O_j < 0$, $O_k > 0$, with two directions shrinking and one expanding.

This classification presents all possible nontrivial cases. Our terminology fits the one used in [41] due to the relation $O_i = 6\kappa k_i K$, ($0 < K = const$), where constants k_i are defined by (2.1.2).

For more details see Appendix B.

2.2.3 True Hamiltonian

Now we can define a generator of an evolution called a true Hamiltonian \mathbb{H} . Making use of (2.2.7), and $O_i = const$ (see [49]), we get

$$\{\mathcal{A}_i, \mathbb{H}\} := \frac{d\mathcal{A}_i}{d\varphi} = -(O_j + O_k), \quad \{O_i, \mathbb{H}\} := \frac{dO_i}{d\varphi} = 0. \quad (2.2.12)$$

The solution to (2.2.12) is easily found to be

$$\mathbb{H} = O_1 O_2 + O_1 O_3 + O_2 O_3. \quad (2.2.13)$$

The true Hamiltonian is defined on the reduced phase space which is devoid of constraints. It generates a flow in the family of volume quantities, enumerated by the evolution parameter.

2.3 Quantum level

2.3.1 Representation of elementary observables

We use the Schrödinger representation for the algebra (2.2.9) defined as

$$O_k \rightarrow \widehat{O}_k f_k(x_k) := \frac{\hbar}{i} \frac{d}{dx_k} f_k(x_k), \quad \mathcal{A}_k \rightarrow \widehat{\mathcal{A}}_k f_k(x_k) := x_k f_k(x_k), \quad k = 1, 2, 3. \quad (2.3.1)$$

One may verify that

$$[\hat{O}_i, \hat{O}_j] = 0, \quad [\hat{\mathcal{A}}_i, \hat{\mathcal{A}}_j] = 0, \quad [\hat{\mathcal{A}}_i, \hat{O}_j] = i\hbar \delta_{ij}. \quad (2.3.2)$$

The representation is defined formally on some dense subspaces of a Hilbert space to be specified later.

2.3.2 Kasner-unlike case

The condition $O_1 O_2 + O_1 O_3 + O_2 O_3 > 0$ is automatically satisfied in this case, because O_1, O_2 and O_3 are of the same sign. To be specific, let us consider (1a); the case (1b) can be done by analogy.

Let us quantize the directional volumes by means of w_i defined in (2.2.8). A standard procedure gives¹

$$\begin{aligned} \hat{w} &:= \frac{3\kappa\gamma\lambda}{2} \left(\hat{O} \cosh(3\kappa\hat{\mathcal{A}}) + \cosh(3\kappa\hat{\mathcal{A}}) \hat{O} \right) = \\ &= -\frac{ia}{2} \left(2 \cosh(bx) \frac{d}{dx} + b \sinh(bx) \right), \end{aligned} \quad (2.3.3)$$

where $a := 3\kappa\gamma\lambda\hbar$ and $b := 3\kappa$, and where we have used the representation for the elementary observables defined by (2.3.1).

In what follows we solve the eigenvalue problem for the operator \hat{w} and identify its domain of self-adjointness.

Let us consider the invertible mapping $L^2(\mathbb{R}, dx) \ni \psi \rightarrow \tilde{U}\psi =: f \in L^2(\mathbb{I}, dy)$ defined by

$$\tilde{U}\psi(x) := \frac{\psi(\ln |\operatorname{tg}^{1/b}(\frac{bx}{2})|)}{\sin^{1/2}(by)} =: f(y), \quad x \in \mathbb{R}, \quad y \in \mathbb{I} := (0, \pi/b). \quad (2.3.4)$$

¹Subscripts of observables are dropped to simplify notation.

We have

$$\begin{aligned}
\langle \psi | \psi \rangle &= \int_{-\infty}^{\infty} \bar{\psi} \psi \, dx \\
&= \int_0^{\frac{\pi}{b}} \bar{\psi}(\ln |\operatorname{tg}^{1/b}(\frac{by}{2})|) \psi(\ln |\operatorname{tg}^{1/b}(\frac{by}{2})|) d(\ln |\operatorname{tg}^{1/b}(\frac{by}{2})|) \\
&= \int_0^{\frac{\pi}{b}} \bar{\psi}(\ln |\operatorname{tg}^{1/b}(\frac{by}{2})|) \psi(\ln |\operatorname{tg}^{1/b}(\frac{by}{2})|) \frac{dy}{\sin(by)} \\
&= \int_0^{\frac{\pi}{b}} \frac{\overline{\psi(\ln |\operatorname{tg}^{1/b}(\frac{by}{2})|)}}{\sin^{1/2}(by)} \frac{\psi(\ln |\operatorname{tg}^{1/b}(\frac{by}{2})|)}{\sin^{1/2}(by)} \, dy = \langle \tilde{U}\psi | \tilde{U}\psi \rangle. \tag{2.3.5}
\end{aligned}$$

Thus, the mapping (2.3.4) is isometric and hence unitary.

Now, let us see how the operator \hat{w} transforms under the unitary map (2.3.4).

The transformation consists of the change of an independent variable

$$x \mapsto y := \frac{2}{b} \arctan(e^{bx}), \tag{2.3.6}$$

which leads to

$$-\frac{ia}{2} \left(2 \cosh(bx) \frac{d}{dx} + b \sinh(bx) \right) \mapsto -ia \frac{d}{dy} + i \frac{ab}{2} \cot(by), \tag{2.3.7}$$

and re-scaling with respect to a dependent variable

$$-ia \frac{d}{dy} + i \frac{ab}{2} \cot(by) \mapsto \sin^{-1/2}(by) \left(-ia \frac{d}{dy} + i \frac{ab}{2} \cot(by) \right) \sin^{1/2}(by) = -ia \frac{d}{dy}. \tag{2.3.8}$$

In the process of mapping

$$\hat{w} \mapsto \tilde{U} \hat{w} \tilde{U}^{-1} = -ia \frac{d}{dy} =: \check{w}, \tag{2.3.9}$$

we have used two identities: $\sin(by) = 1/\cosh(bx)$ and $\sinh(bx) = -\cot(by)$.

Since $w > 0$ (for $O > 0$), we assume that the spectrum of \check{w} consists of positive eigenvalues. To implement this assumption, we define $\check{w} := \sqrt{\check{w}^2}$ and consider the

eigenvalue problem

$$-a^2 \frac{d^2}{dy^2} f_\nu = \nu^2 f_\nu, \quad y \in (0, \pi/b). \quad (2.3.10)$$

There are two independent solutions for each value of ν^2 (where $\nu \in \mathbb{R}$), namely: $\sin(\frac{\nu}{a}y)$ and $\cos(\frac{\nu}{a}y)$. Removing this degeneracy leads to required positive eigenvalues of \check{w} . We achieve that in a standard way by requiring that the eigenvectors vanish at the boundaries, i.e, at $y = 0$ and $y = \pi/b$. As the result we get the following spectrum

$$f_\nu = N \sin\left(\frac{\nu}{a}y\right), \quad \nu^2 = (nab)^2, \quad n = 0, 1, 2, \dots \quad (2.3.11)$$

It should be noted that for $n = 0$, the eigenvector is a null state and thus the lowest eigenvalue is $\nu^2 = (ab)^2$. Next, we define the Hilbert space to be the closure of the span of the eigenvectors (2.3.11). The operator $\check{w}^2 = -a^2 \frac{d^2}{dy^2}$ is essentially self-adjoint on this span by the construction. Due to the spectral theorem [43] we may define an essentially self-adjoint operator $\check{w} = \sqrt{-a^2 \frac{d^2}{dy^2}}$ as follows

$$\check{w} f_\nu := \nu f_\nu, \quad \nu = ab, 2ab, 3ab, \dots \quad (2.3.12)$$

We have considered the case $w > 0$. The case $w < 0$ does not require changing of the Hilbert space. The replacement $\hat{w} \mapsto -\hat{w}$ leads to $\nu \mapsto -\nu$.

Finally, we find that the inverse mapping from $L^2(\mathbb{I}, dy)$ to $L^2(\mathbb{R}, dx)$ for the eigenvectors of \check{w} yields

$$\sin\left(\frac{\nu}{a}y\right) = f_\nu(y) \mapsto \tilde{U}^{-1} f_\nu(y) := \psi_\nu(x) = \frac{\sin\left(\frac{2\nu}{ab}\text{arctg}(e^{bx})\right)}{\cosh^{1/2}(bx)}. \quad (2.3.13)$$

2.3.3 Kasner-like case

In the case (2a), the conditions $O_1 O_2 + O_1 O_3 + O_2 O_3 > 0$ with $O_1 < 0, O_2 > 0, O_3 > 0$ are satisfied in the following domains² for O_k

$$O_1 \in (-d_1, 0), \quad O_2 \in (d_2, \infty), \quad O_3 \in (d_3, \infty), \quad (2.3.14)$$

where $d_2 > d_1$, and where $d_3 = d_1 d_2 / (d_2 - d_1)$ so $d_3 > d_1$. The full phase space sector of the Kasner-like evolution is defined as the union

$$\bigcup_{0 < d_1 < d_2} (-d_1, 0) \times (d_2, \infty) \times (d_3, \infty) \quad (2.3.15)$$

In the case of O_2 and O_3 , the restrictions for domains (2.3.14) translate into the restrictions for the corresponding domains for the observables w_2 and w_3 , due to (2.2.8), and read

$$w_2 \in (D_2, \infty), \quad w_3 \in (D_3, \infty), \quad (2.3.16)$$

where $D_2 = \kappa\gamma\lambda d_2$ and $D_3 = \kappa\gamma\lambda d_3$. Thus, quantization of the w_2 and w_3 observables can be done by analogy to the Kasner-unlike case. The spectra of the operators \hat{w}_2 and \hat{w}_3 are almost the same as the spectrum defined by (2.3.12) with the only difference that now $\nu > D_2$ and $\nu > D_3$, respectively³.

The case of w_1 requires special treatment. Let us redefine the elementary observables corresponding to the 1-st direction as follows

$$\Omega_1 := -\frac{O_1}{b \cosh(b\mathcal{A}_1)}, \quad \Omega_2 := \sinh(b\mathcal{A}_1). \quad (2.3.17)$$

The transformation (2.3.17) is canonical, since $\{\Omega_1, \Omega_2\} = 1$, and invertible. The domains transform as follows

$$O_1 \in (-d_1, 0), \quad \mathcal{A}_1 \in \mathbb{R} \quad \longrightarrow \quad \Omega_1 \in (0, d_1/b) =: (0, D_1), \quad \Omega_2 \in \mathbb{R}. \quad (2.3.18)$$

²The case (2b) can be done by analogy.

³Spectra are insensitive to unitary transformations.

The observable v_1 in terms of redefined observables reads

$$v_1 = \frac{ab}{\hbar} \Omega_1 (1 + \Omega_2^2), \quad v_1 \in (0, \infty), \quad (2.3.19)$$

where $ab/\hbar = 12\pi G\gamma\lambda$. To quantize observables Ω_1 and Ω_2 we use the Schrödinger representation

$$\Omega_2 \rightarrow \hat{\Omega}_2 f(x) := -i\hbar\partial_x f(x), \quad \Omega_1 \rightarrow \hat{\Omega}_1 f(x) := xf(x), \quad f \in L^2(0, D_1). \quad (2.3.20)$$

Let us find an explicit form for the operator $\frac{ab}{\hbar}(\hat{\Omega}_1 + \widehat{\Omega_1\Omega_2^2})$, corresponding to (2.3.19). Since $\Omega_1 > 0$, the following classical equality holds

$$\Omega_1\Omega_2^2 = \Omega_1^k \cdot \Omega_2 \cdot \Omega_1^{1-k-m} \cdot \Omega_2 \cdot \Omega_1^m, \quad (2.3.21)$$

where $m, k \in \mathbb{R}$. This may lead to many operator orderings at the quantum level. This issue is further discussed in the appendix.

We propose the following mapping (we set $\hbar = 1$)

$$\begin{aligned} \Omega_1\Omega_2^2 \rightarrow \widehat{\Omega_1\Omega_2^2} &:= \frac{1}{2} \left(\hat{\Omega}_1^k \hat{\Omega}_2 \hat{\Omega}_1^{1-k-m} \hat{\Omega}_2 \hat{\Omega}_1^m + \hat{\Omega}_1^m \hat{\Omega}_2 \hat{\Omega}_1^{1-k-m} \hat{\Omega}_2 \hat{\Omega}_1^k \right) = \\ &= -x\partial_{xx}^2 - \partial_x + m k x^{-1}, \end{aligned} \quad (2.3.22)$$

which formally ensures the symmetricity of $\widehat{\Omega_1\Omega_2^2}$. The second equality in (2.3.22) may be verified via direct calculations.

Now, we define the following unitary transformation W

$$L^2([0, D_1], dx) \ni f(x) \mapsto Wf(x) := \sqrt{\frac{y}{2}} f\left(\frac{y^2}{4}\right) \in L^2([0, 2\sqrt{D_1}], dy). \quad (2.3.23)$$

One may verify that we have

$$W\partial_x W^\dagger = \frac{2}{y}\partial_y - \frac{1}{y^2}, \quad W\partial_{xx}^2 W^\dagger = \frac{4}{y^2}\partial_{yy}^2 - \frac{8}{y^2}\partial_y + \frac{5}{y^4}. \quad (2.3.24)$$

Thus, the operator W transforms (2.3.22) into

$$-\partial_{yy}^2 + \frac{1}{y^2} \left(4mk - \frac{1}{4} \right). \quad (2.3.25)$$

The eigenvalue problem for $\widehat{\Omega}_1 + \widehat{\Omega}_1 \Omega_2^2$ reads

$$\left(-\partial_{yy}^2 + \frac{1}{y^2} \left(4mk - \frac{1}{4} \right) + \frac{y^2}{4} \right) \Phi = \nu \Phi. \quad (2.3.26)$$

Now, we can see an advantage of the chosen ordering prescription (2.3.22). It enables finding a very simple form of the volume operator. Taking $k = m = 1/4$ turns (2.3.26) into

$$\left(-\partial_{yy}^2 + \frac{y^2}{4} - \nu \right) \Phi = 0. \quad (2.3.27)$$

The problem is mathematically equivalent to the one dimensional harmonic oscillator in a “box” with an edge equal to $2\sqrt{D_1}$. There are two independent solutions for a given ν

$$\Phi_{\nu,1} = N_1 e^{-y^2/4} {}_1F_1 \left(-\frac{1}{2}\nu + \frac{1}{4}, \frac{1}{2}, \frac{y^2}{2} \right), \quad (2.3.28)$$

$$\Phi_{\nu,2} = N_2 y e^{-y^2/4} {}_1F_1 \left(-\frac{1}{2}\nu + \frac{3}{4}, \frac{3}{2}, \frac{y^2}{2} \right), \quad (2.3.29)$$

where ${}_1F_1$ is a hypergeometric confluent function, $\Phi_{\nu,1}$ and $\Phi_{\nu,2}$ are even and odd cylindrical functions, respectively. A standard condition for the symmetricity of the operator defining the eigenvalue problem (2.3.27) leads to the vanishing of the wave functions at the boundaries (as the box defines the entire size of the 1-st direction).

The solution (after retrieving of \hbar and ab) reads⁴.

$$\Phi = N y e^{-\frac{y^2}{4\hbar}} {}_1F_1 \left(-\frac{1}{2} \frac{\nu}{ab} + \frac{3}{4}, \frac{3}{2}, \frac{y^2}{2\hbar} \right). \quad (2.3.30)$$

⁴We ignore the solution $\Phi_{\nu,1}$ because it cannot vanish at $y = 0$.

The solution (2.3.30) vanishes at $y = 0$ as Φ is an odd function. The requirement of vanishing at $y = 2\sqrt{D_1}$ leads to the equation

$${}_1F_1\left(-\frac{1}{2}\frac{\nu}{ab\hbar} + \frac{3}{4}, \frac{3}{2}, \frac{2D_1}{\hbar}\right) = 0. \quad (2.3.31)$$

An explicit form of (2.3.31) reads

$$\sum_{n=0}^{\infty} \frac{(-\frac{1}{2}\frac{\nu}{ab} + \frac{3}{4})_n}{(\frac{3}{2})_n} \left(\frac{2D_1}{\hbar}\right)^n = 0, \quad (2.3.32)$$

where $(a)_n = a(a+1)\dots(a+n-1)$. It results from (2.3.32) that the eigenvalues must satisfy the condition: $\nu \geq ab$.

2.3.4 Volume operator

Classically we have

$$V = |w_1 w_2 w_3|^{1/3}. \quad (2.3.33)$$

One may verify that v_k Poisson commute and \hat{v}_k commute, so we can take

$$\widehat{V}^3 := \hat{v}_1 \hat{v}_2 \hat{v}_3 = |\hat{w}_1 \hat{w}_2 \hat{w}_3|. \quad (2.3.34)$$

The eigenfunctions of the operator $\hat{w}_1 \hat{w}_2 \hat{w}_3$ have the form

$F^{\lambda_1, \lambda_2, \lambda_3} := f_1^{\lambda_1}(x_1) f_2^{\lambda_2}(x_2) f_3^{\lambda_3}(x_3)$, where $f_i^{\lambda_i}(x_i)$ is an eigenvector of \hat{w}_i with eigenvalue λ_i . The closure of the span of $F^{\lambda_1, \lambda_2, \lambda_3}$ is a Hilbert space, in which \widehat{V}^3 is a self-adjoint operator (by construction).

Due to the spectral theorem on self-adjoint operators [43], we have

$$V = (V^3)^{1/3} \longrightarrow \widehat{V} F^{\lambda_1, \lambda_2, \lambda_3} := \square F^{\lambda_1, \lambda_2, \lambda_3}, \quad (2.3.35)$$

where

$$\square := |\lambda_1 \lambda_2 \lambda_3|^{1/3}. \quad (2.3.36)$$

Kasner-unlike case

In the Kasner-unlike case we use the formula (2.3.12) to get

$$\square = |n_1 n_2 n_3|^{1/3} ab, \quad n_1, n_2, n_3 \in 1, 2, 3, \dots, \quad (2.3.37)$$

which shows that the spectrum of the volume operator does not have equally distant levels. The volume \square equal to zero is not in the spectrum. There exist a quantum of the volume which equals $\Delta := ab = 12\pi G\gamma\lambda\hbar$, and which defines the lowest value in the spectrum.

Kasner-like case

The spectrum in this case reads

$$\square := \bigcup_{0 < d_1 < d_2} \square_{d_1, d_2}, \quad \square_{d_1, d_2} := \{\lambda_{d_1} \lambda_{d_2} \lambda_{d_3} \mid d_3 = d_1 d_2 / (d_2 - d_1)\}, \quad (2.3.38)$$

where λ_{d_1} is any value subject to the condition (2.3.32), $\lambda_{d_2} > D_2$ and $\lambda_{d_3} > D_3$ are given by (2.3.12). The volume \square equal to zero is not in the spectrum.

2.3.5 Evolution

In this section we ignore the restrictions concerning the domains of O_1 , O_2 and O_3 , and we assume that the Hilbert space of the system is $L^2(\mathbb{R}^3, dx dy dz)$. An inclusion of the restrictions would complicate the calculations without bringing any qualitative change into the picture of evolution.

The generator of evolution determined in (2.2.13) may be formally quantized, due to (2.3.1), as follows

$$\mathbb{H} \mapsto \hat{\mathbb{H}} = -\hbar^2 (\partial_y \partial_z + \partial_x \partial_z + \partial_x \partial_y). \quad (2.3.39)$$

Since it is self-adjoint in $L^2(\mathbb{R}^3, dx dy dz)$, a quantum evolution can be defined by an unitary operator

$$U = e^{-i\hbar\tau(\partial_y\partial_z + \partial_x\partial_z + \partial_x\partial_y)}, \quad \tau \in \mathbb{R}. \quad (2.3.40)$$

Let us study an evolution of the expectation value of the directional volume \hat{v}_1

$$\langle \psi | U^{-1} \hat{v}_1 U | \psi \rangle \quad (2.3.41)$$

Since \hat{v}_1 does not depend on y and z , we simplify our considerations by taking

$$U_1 = e^{-i\hbar\tau(\partial_z + \partial_y)\partial_x}. \quad (2.3.42)$$

If we are interested in the action of U_1 on the functions $f(x) \in L^2(\mathbb{R}, dx)$, then the derivatives $-i\frac{d}{dy}$ and $-i\frac{d}{dz}$ occurring in U_1 commute and, being self-adjoint, lead finally to real numbers. Let us call them k_y and k_z , respectively, and let us introduce the parameter $k = k_y + k_z$. Hence, U_1 further simplifies and reads

$$U_1 = e^{k\hbar\tau\partial_x}. \quad (2.3.43)$$

The action of U_1 on $f(x)$ reads

$$U_1 f(x) = f(x + k\hbar\tau). \quad (2.3.44)$$

We recall that under the unitary mapping $L^2(\mathbb{R}, dx) \mapsto L^2(\mathbb{I}, dy)$, defined by (2.3.4), the operator \hat{v}_1 becomes $-ia\frac{d}{dy}$ on $L^2(\mathbb{I}, dy)$. Now, let us study an action of operator U_1 on the functions $\varphi(y) \in L^2(\mathbb{I}, dy)$. Straightforward calculation leads to

$$L^2(\mathbb{I}, y) \ni \varphi(y) \mapsto \frac{\varphi(\frac{2}{b} \arctan(e^{bx}))}{\cosh^{1/2}(bx)} \in L^2(\mathbb{R}, x), \quad (2.3.45)$$

and we have

$$U_1 \frac{\varphi(\frac{2}{b} \arctan(e^{bx}))}{\cosh^{1/2}(bx)} = \frac{\varphi(\frac{2}{b} \arctan(e^{bx+bk\hbar\tau}))}{\cosh^{1/2}(bx + bk\hbar\tau)} \quad (2.3.46)$$

The transformation \tilde{U}^{-1} gives

$$\frac{\varphi(\frac{2}{b} \arctan(e^{bx+bk\hbar\tau}))}{\cosh^{1/2}(bx+bk\hbar\tau)} \mapsto \frac{\varphi(\frac{2}{b} \arctan(e^{bk\hbar\tau} \tan(\frac{by}{2})))}{\sqrt{\frac{1}{2} \sin(by)(\tan(\frac{by}{2})e^{bk\hbar\tau} + \cot(\frac{by}{2})e^{-bk\hbar\tau})}} =: \varphi_\tau(y), \quad (2.3.47)$$

where $\varphi_{\tau=0}(y) = \varphi(y)$. Now, we observe that the symmetry condition

$$\langle \varphi_\tau(y) | \hat{v}_1 \varphi_\tau(y) \rangle = \langle \hat{v}_1 \varphi_\tau(y) | \varphi_\tau(y) \rangle \quad (2.3.48)$$

leads to

$$\overline{\varphi}_\tau\left(\frac{\pi}{b}\right)\varphi_\tau\left(\frac{\pi}{b}\right) - \overline{\varphi}_\tau(0)\varphi_\tau(0) = 0. \quad (2.3.49)$$

We use the result (2.3.47) to calculate the limits

$$\lim_{y \rightarrow 0} \varphi_\tau(y) = e^{\frac{bk\hbar\tau}{2}} \varphi_0(0), \quad \lim_{y \rightarrow \frac{\pi}{b}} \varphi_\tau(y) = e^{-\frac{bk\hbar\tau}{2}} \varphi_0\left(\frac{\pi}{b}\right), \quad (2.3.50)$$

which turns (2.3.49) into

$$\overline{\varphi}_0\left(\frac{\pi}{b}\right)\varphi_0\left(\frac{\pi}{b}\right)e^{-bk\hbar\tau} - \overline{\varphi}_0(0)\varphi_0(0)e^{bk\hbar\tau} = 0. \quad (2.3.51)$$

It is clear that (2.3.51) can be satisfied $\forall \tau$ iff $\varphi_0(\frac{\pi}{b}) = 0 = \varphi_0(0)$. States with such a property belong to the domain of \check{w} defined by (2.3.12).

In order to construct the “evolving states” that vanish at the boundaries, consider the basis vectors $f_n(y) = e^{i2bny}$. Then, $f_n(y) - f_m(y)$ satisfy the condition (2.3.51). Making use of (2.3.47) we get

$$f_n(y, \tau) = \left(\frac{i - e^{bk\hbar\tau} \tan(\frac{by}{2})}{i + e^{bk\hbar\tau} \tan(\frac{by}{2})} \right)^{2n} \sqrt{\frac{1 + \tan^2(\frac{by}{2})}{e^{-bk\hbar\tau} + e^{bk\hbar\tau} \tan^2(\frac{by}{2})}}, \quad (2.3.52)$$

where $f_n(y, \tau) := f_{n,\tau}(y)$. Moreover we have

$$\begin{aligned} -ia \frac{d}{dy} f_n(y, \tau) &= -i \frac{ab}{2} \left(1 + \tan^2\left(\frac{by}{2}\right)\right) f_n(y, \tau) \frac{1}{1 + e^{2bk\hbar\tau} \tan^2\left(\frac{by}{2}\right)} \times \\ &\quad \times \left(\frac{(1 - e^{2bk\hbar\tau}) \tan\left(\frac{by}{2}\right)}{1 + \tan^2\left(\frac{by}{2}\right)} + i4ne^{bk\hbar\tau} \right). \end{aligned} \quad (2.3.53)$$

Using the substitution $x = \tan(\frac{by}{2})$ we get

$$\begin{aligned} \langle f_m | -ia \frac{d}{dy} f_n \rangle &= \\ -ia \int_0^\infty \left(\frac{i - e^{bk\hbar\tau}x}{i + e^{bk\hbar\tau}x} \right)^{2(n-m)} \frac{(e^{-bk\hbar\tau} - e^{bk\hbar\tau})x}{(e^{-bk\hbar\tau} + e^{bk\hbar\tau}x^2)^2} dx \\ + 4an \int_0^\infty \left(\frac{i - e^{bk\hbar\tau}x}{i + e^{bk\hbar\tau}x} \right)^{2(n-m)} \frac{1 + x^2}{(e^{-bk\hbar\tau} + e^{bk\hbar\tau}x^2)^2} dx. \end{aligned} \quad (2.3.54)$$

Another substitution $z = e^{bk\hbar\tau}x$ leads to

$$\begin{aligned} \langle f_m | -ia \frac{d}{dy} f_n \rangle &= \\ -ia(e^{-bk\hbar\tau} - e^{bk\hbar\tau}) \int_0^\infty \left(\frac{i - z}{i + z} \right)^{2(n-m)} \frac{z}{(1 + z^2)^2} dz \\ + 4an \int_0^\infty \left(\frac{i - z}{i + z} \right)^{2(n-m)} \frac{e^{bk\hbar\tau} + e^{-bk\hbar\tau}z^2}{(1 + z^2)^2} dz \end{aligned} \quad (2.3.55)$$

Finally, we obtain

$$\langle f_m | -ia \frac{d}{dy} f_n \rangle = \begin{cases} \frac{ia}{4(n-m)^2-1}(1 - 8n(n-m)) \sinh(bk\hbar\tau), & n \neq m \\ ia \sinh(bk\hbar\tau) + 2\pi na \cosh(bk\hbar\tau), & n = m. \end{cases} \quad (2.3.56)$$

Now, let us introduce $g_{nm}(y, \tau) := \frac{f_n(y, \tau) - f_m(y, \tau)}{\sqrt{\frac{2\pi}{b}}}$ so that $\|g_{nm}\| = 1$. One has

$$\langle g_{nm} | -ia \frac{d}{dy} g_{nm} \rangle = (n + m)ab \cosh(bk\hbar\tau) = \frac{n + m}{2} \Delta \cosh(bk\hbar\tau). \quad (2.3.57)$$

The expectation value of the operator (2.3.57), defining the volume operator, is similar to the classical form (2.2.8). The vectors g_{nm} may be used in the construction of a basis of the space of states such that $\varphi_0(\frac{\pi}{b}) = 0 = \varphi_0(0)$.

2.3.6 Summary

As in the FRW case, resolution of the singularity in the Bianchi I model is due to the loop modification of the Hamiltonian at the classical level. This modification is parameterized by a free continuous parameter λ .

The spectrum of the volume operator, parameterized by λ , is bounded from below and discrete. An evolution of the expectation value of the volume operator is similar to the classical case. We have presented the evolution of only a single directional volume operator. One may try to generalize this procedure to the total volume operator. In the case of the Kasner-like analyzes of dynamics are complicated.

We introduced the so-called true Hamiltonian which proves an independence of the spectrum of the volume operator on the evolution.

Conclusions

Firstly, in the nonstandard LQC the results are obtained directly on the physical Hilbert space. Secondly, our nonstandard loop quantum cosmology, successfully applied so far to the FRW and Bianchi I models, seems to be highly efficient. For example, only analytical calculations are needed to obtain the results.

Turning the Big Bang into the Big Bounce in our method is due to the modification of the Hamiltonian at the classical level by making use of the loop geometry. The modification is parameterized by a continuous parameter λ , which value is not known.

In both considered models the spectrum of the volume operators, parameterized by λ , are bounded from below and discrete. An evolution of the expectation values of the volume operators are similar to the classical cases.

In the Bianchi I model, the phase space of the system is divided into the two distinct regions: the Kasner-like and the Kasner-unlike. Domains, spectra and eigenvectors of self-adjoint directional volumes, and total volume operators were identified in the Kasner-unlike case. The peculiarity of the Kasner-like case was identified due to complicated boundary of the phase space region. We propose to overcome this problem by dividing this region further into smaller regions, but with simpler boundaries. Given a small subregion for the Kasner-like case, we propose a canonical redefinition of phase space coordinates in such a way, that we can arrive at relatively simple form

of volume operator and at the same time can simply encode the boundary of the region into the Schrödinger representation. Then, from a number of different operator orderings the simplest one was chosen. Domain, spectrum and eigenvectors of the volume operator was founded. The spectrum is given in an implicit form in terms of special functions.

Discreteness of space at the quantum level may lead to a foamy structure of spacetime at the semi-classical level. The discreteness is also specific to the FRW case [38]. The difference is that in the Bianchi I case the variety of possible quanta of a volume is much richer. On the other hand, the Bianchi type cosmology seems to be more realistic than the FRW case, near the cosmological singularity. Thus, an expected foamy structure of space may better fit cosmological data. Various forms of discreteness of space may underly many approaches in fundamental physics. So its examination may be valuable.

As we know λ is a free parameter. Without specific choice of λ , the Big Bounce may occur at any low or high density. The former case (big λ) contradicts the data of observational cosmology (there was no Big Bounce in the near past) and leads to weakly controlled modification of the expression for the curvature F_{ab}^k , i.e. gravitational part of the Hamiltonian (see Appendix A). On the other hand the latter case (small λ) gives much better approximation for the classical Hamiltonian (see Appendix A), but may easily lead to densities much higher than the Planck scale density, where the classical formalism is believed to be inadequate. Finding specific value of the parameter λ , i.e. the energy scale specific to the Big Bounce is an open problem. It may happen, that the value of the parameter λ cannot be determined, for some reason, theoretically. The story may turn out to be similar to the case

of the short-range repulsive part of the potential of the nucleon-nucleon interaction introduced to explain the scattering data [54] and the nuclear matter saturation of energy [55]. In such a case λ will become a phenomenological variable parameterizing our ignorance of microscopic properties of the Universe. Fortunately, there is a rapidly growing number of data coming from observational cosmology that may be useful in this context. The cosmic projects for the detection of gamma ray bursts may reveal that the velocity of cosmic photons depend on their wave lengths, which may be ascribed to the foamy nature of spacetime [56, 57, 58]. Such dependence is weak, but may sum up to give a measurable effect in the case of photons travelling over cosmological distances across the Universe [59]. Presently, available data suggest that such dispersion effects do not occur up to the energy scale 5×10^{17} GeV [60] so such effects may be present, but at higher energies. Another way to determine the phenomenological value of the parameter λ is the detection of the primordial gravitational waves created at the Big Bounce [61, 62, 63, 64].

In our method an evolution parameter φ does not belong to the physical phase space, contrary to the standard LQC. Thus, it stays classical during the quantization process as well. At quantum level of the Bianchi I model, for the first time in our method, the so-called true Hamiltonian was introduced. It generates a flow in the family of volume quantities, enumerated by an evolution parameter. Having the true Hamiltonian, we could introduce an unitary operator with the evolution parameter $\tau \in \mathbb{R}$.

It is clear that the next step, in the road to understand an early Universe, is the nonstandard LQC quantization of the Bianchi II cosmological model.

Appendix A

Holonomy corrections

The curvature of $SU(2)$ connection $F_{ab}^k = \partial_a A_b^k - \partial_b A_a^k + \epsilon_{ij}^k A_a^i A_b^j$, entering the expression (1.2.2) for the gravitational part of the Hamiltonian, can be expressed in terms of holonomies. Using the mean-value and Stokes' theorems we have

$$\tau_k F_{ab}^k(\vec{x}) \approx \frac{1}{s_{ab}^\sigma} \int_\sigma \tau_k F_{cd}^k dx^c \wedge dx^d \approx \frac{1}{s_{ab}^\sigma} \left(\mathcal{P} \exp \left(\oint_{\partial\sigma} \tau_k A_c^k dx^c \right) - 1 \right), \quad (\text{A.0.1})$$

where $\partial\sigma$ is the boundary of a small surface σ with center at \vec{x} , and where $s_{ab}^\sigma := \int_\sigma dx^a \wedge dx^b$. The expression for F_{ab}^k is exact but in the limit when we shrink the area enclosed by the loop $\partial\sigma$ to zero. If we choose $\partial\sigma$ in the form of the square \square_{ij} with sides length λ , the expression for a small value of $\lambda = \mu_0$ has the form [65]

$$F_{ab}^k(\mu_0) = \lim_{\lambda \rightarrow \mu_0} \left\{ -2 \operatorname{Tr} \left(\frac{h_{\square_{ij}}^{(\lambda)} - 1}{\lambda^2 V_o^{2/3}} \right) \tau^k {}^o\omega_a^i {}^o\omega_a^j + \frac{\mathcal{O}(\lambda^4)}{\lambda^2} \right\}, \quad (\text{A.0.2})$$

and we have

$$F_{ab}^k = \lim_{\mu_0 \rightarrow 0} F_{ab}^k(\mu_0). \quad (\text{A.0.3})$$

In the standard LQC the $\mathcal{O}(\lambda^4)$ holonomy corrections are ignored (see, e.g. [22, 23]). It was found in [65, 66] that including higher order corrections leads to new curvature singularities different from the initial singularity and increases an ambiguity

problem of loop cosmology. However, the holonomy corrections do not change the result that the Big Bounce is a consequence of the loopy nature of geometry [67].

Taking only the first term of (A.0.2) leads to the simplest modification of gravity, but may be insufficient for the description of the inflationary phase. The choice of μ_0 based on the expectation that the Big Bounce should occur at the Planck scale [22] has little justification [36]. The significance of Planck's scale for quantum gravity seems to be rather a belief than proved result (see, e.g. [68]). Heuristic reasoning playing game at the same time with Heisenberg's uncertainty principle, Schwarzschild's radius and process of measurement cannot replace a proof (see, e.g. [69]).

Appendix B

Justification for using observables to classify phase space

B.1 Nonregularized case

The nonregularized case means that we do not modify general relativity by loop geometry (loops of finite length). For this case one has¹

$$O_i = \frac{1}{\kappa\gamma} v_i \beta_i, \quad (\text{B.1.1})$$

where

$$v_i := (a_j a_k L_j L_k)^{3/2}, \quad \beta_i := \frac{\dot{a}_i \gamma}{(a_j a_k L_j L_k)^{1/2}}. \quad (\text{B.1.2})$$

It is clear that

$$O_i = \frac{1}{\kappa} a_i a_j a_k L_i L_j L_k \frac{\dot{a}_i}{a_i} =: \frac{V}{\kappa} H_i, \quad (\text{B.1.3})$$

which leads to

$$H_k = \frac{\kappa}{V} O_k \quad (\text{B.1.4})$$

where $H_k := \dot{a}_k/a_k$ is a directional Hubble parameter in the k -th direction. In what follows we use H_k to describe contraction or expansion of spacetime. It results from

¹obtained from (2.2.1) in the limit $\lambda \rightarrow 0$

(B.1.4) that classical dynamics of our system in the nonregularized case can be described in terms of the observables O_k .

B.2 Regularized case

In this case we modify gravity by loop geometry, due to (2.2.6), we have

$$v_i = \kappa\gamma\lambda|O_i| \cosh(3\kappa((O_j + O_k)\varphi - A_i)) \quad (\text{B.2.1})$$

so we get

$$\frac{\dot{v}_i}{v_i} = 3\kappa(O_j + O_k) \tanh(3\kappa((O_j + O_k)\varphi - A_i)) \dot{\varphi} \quad (\text{B.2.2})$$

where $\dot{\varphi} = \frac{1}{2} \frac{1}{V}$. On the other hand we have

$$\frac{\dot{v}_i}{v_i} = \frac{3}{2}(H_j + H_k). \quad (\text{B.2.3})$$

Comparing (B.2.2) and (B.2.3) we obtain

$$H_j + H_k = \frac{\kappa}{V}(O_j + O_k) \tanh(3\kappa((O_j + O_k)\varphi - A_i)). \quad (\text{B.2.4})$$

Denoting the moment of occurring a bounce by φ_i^B , defined by

$$A_i = (O_j + O_k)\varphi_i^B, \quad (\text{B.2.5})$$

we obtain the formula

$$H_j + H_k = \frac{\kappa}{V}(O_j + O_k) \tanh(3\kappa(O_j + O_k)(\varphi - \varphi_i^B)). \quad (\text{B.2.6})$$

For the purpose of interpretation it is convenient to rewrite (B.2.6) in different form. Since $\cosh(x)^2 - \sinh(x)^2 = 1$, we have

$$\tanh(x) = \pm \sqrt{1 - \frac{1}{\cosh^2(x)}}. \quad (\text{B.2.7})$$

In the case of expanding universe, $\varphi > \varphi_i^B$, we have the expression

$$\tanh(3\kappa(O_j + O_k)(\phi - \phi_i^B)) = \sqrt{1 - \frac{1}{\cosh^2(3\kappa(O_j + O_k)(\varphi - \varphi_i^B))}}. \quad (\text{B.2.8})$$

It results from (B.2.1) and (B.2.5) that

$$v_i = \kappa\gamma\lambda O_i \cosh(3\kappa(O_j + O_k)(\varphi - \varphi_i^B)). \quad (\text{B.2.9})$$

Since $v_i^B = \kappa\gamma\lambda O_i$ (directional volume at the i-th bounce), we have

$$\frac{1}{\cosh(3\kappa(O_j + O_k)(\varphi - \varphi_i^B))} = \frac{v_i^B}{v_i}, \quad (\text{B.2.10})$$

which means that

$$\tanh(3\kappa(O_j + O_k)(\varphi - \varphi_i^B)) = \sqrt{1 - \left(\frac{v_i^B}{v_i}\right)^2}. \quad (\text{B.2.11})$$

Inserting (B.2.11) into (B.2.6) gives finally

$$H_j + H_k = \frac{\kappa}{V}(O_j + O_k) \sqrt{1 - \left(\frac{v_i^B}{v_i}\right)^2}. \quad (\text{B.2.12})$$

It results from (B.2.12) that for very large v_i , comparing to v_i^B , we can apply the approximation

$$H_j + H_k = \frac{\kappa}{V}(O_j + O_k), \quad (\text{B.2.13})$$

which finally leads to

$$H_k = \frac{\kappa}{V} O_k. \quad (\text{B.2.14})$$

Comparing (B.1.4) and (B.2.14) one can see that also for the regularized case the structure of the classical phase space may be described in terms of O_k observables, but only when we consider the Universe far away from the Big Bounce ($v_i \gg v_i^B$). However, for our analyzes that limitation does not matter.

Appendix C

Non-uniqueness in quantization of the Bianchi I

It is clear that quantum cosmology calculations are plagued by quantization ambiguities. For example, there exists a huge freedom in ordering of elementary operators defining compound observables, which may lead to different quantum operators. Classical commutativity of variables does not extend to corresponding quantum operators. Other ambiguities are discussed below. Such ambiguities can be largely reduced when some quantum data from cosmological observations become available. Confrontation of theoretical predictions against these data would enable finding realistic quantum cosmology models.

C.1 Unitarily non-equivalent volume operators

In both Kasner-like and Kasner-unlike cases, we have reduced the Hilbert space by removing the double degeneracy of eigenvalues for the volume operators (see the discussion after equations (2.3.10) and (2.3.27)). We have used the “natural” condition that the wave function should vanish at the boundaries of an interval. However, there are also other mathematically well-defined choices for the boundary conditions. We

will demonstrate this non-uniqueness for the Kasner-unlike case. Similar reasoning applies to another case.

Let us begin with the equation (2.3.10)

$$-a^2 \frac{d^2}{dy^2} f = \nu^2 f, \quad y \in (0, \pi/b), \quad (\text{C.1.1})$$

which has the solution

$$f_\nu = N_1 \sin\left(\frac{\nu}{a}y\right) + N_2 \cos\left(\frac{\nu}{a}y\right), \quad N_1, N_2 \in \mathbb{C}, \quad (\text{C.1.2})$$

for each value of $\nu \in \mathbb{R}_+$ ($\nu \mapsto -\nu$ does not produce any new space of solutions). Our task is the determination of self-adjointness of $\check{w} := \sqrt{-a^2 \frac{d^2}{dy^2}}$ and removing the double degeneracy of eigenvalues. The symmetricity condition reads

$$\int_I \bar{f} f'' = \bar{f} f' \Big|_0^{\pi/b} - \bar{f}' f \Big|_0^{\pi/b} + \int_I \bar{f}'' f. \quad (\text{C.1.3})$$

We can set:

- $f(0) = f(\pi/b) = 0 \Rightarrow f_\nu = \sin\left(\frac{\nu}{a}y\right), \quad \nu = ab, 2ab, 3ab, \dots$
- $f'(0) = f'(\pi/b) = 0 \Rightarrow f_\nu = \cos\left(\frac{\nu}{a}y\right), \quad \nu = 0, ab, 2ab, 3ab, \dots$
- $f(0) = f'(\pi/b) = 0 \Rightarrow f_\nu = \sin\left(\frac{\nu}{a}y\right), \quad \nu = \frac{1}{2}ab, \frac{3}{2}ab, \frac{5}{2}ab, \dots$

where $ab = 12\pi\hbar G\gamma\lambda$. All these choices are non-equivalent, since they lead to different spectra.

C.2 Standard quantization

Let us change the coordinates of the Kasner-like sector phase space (Ω_1, Ω_2) , defined by (2.3.17), into a new canonical pair as follows

$$X := \sqrt{2\Omega_1} \quad \text{and} \quad P := \Omega_2 \sqrt{2\Omega_1}, \quad (\text{C.2.1})$$

where

$$(X, P) \in (0, \sqrt{2d_1/b}) \times \mathbb{R}, \quad \{X, P\} = 1. \quad (\text{C.2.2})$$

In the new variables the volume (2.3.19) reads

$$\frac{1}{4\pi G\gamma\lambda} v_1 = \frac{1}{2}P^2 + \frac{1}{2}X^2. \quad (\text{C.2.3})$$

Thus, in these variables the volume has a form of the Hamiltonian of the harmonic oscillator in a “box” $(0, \sqrt{2d_1/b})$.

In the Schrödinger representation, i.e. $\hat{X} := x$ and $\hat{P} := -i\hbar\partial_x$, a standard quantization yields

$$\frac{1}{4\pi G\gamma\lambda} \hat{v} = -\frac{\hbar^2}{2}\partial_{xx}^2 + \frac{1}{2}x^2, \quad (\text{C.2.4})$$

which corresponds to the “nonstandard” quantization (2.3.26) with the parameters $m = k = 1/4$ and $y = \sqrt{2}x$ (with $\hbar = 1$).

Thus, we can see that the prescription defined by (2.3.21) and (2.3.22) includes not only a standard prescription, but many others. As an illustration only one, corresponding to the well known harmonic oscillator, has been completed.

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